RESEARCH CENTER

FIELD

Activity Report 2016

Section Scientific Foundations

Edition: 2017-08-25

Algorithmics, Programming, Software and Architecture

Applied Mathematics, Computation and Simulation

DIGITAL HEALTH, BIOLOGY AND EARTH

NETWORKS, SYSTEMS AND SERVICES, DISTRIBUTED COMPUTING

PERCEPTION, COGNITION AND INTERACTION

ANTIQUE Project-Team

3. Research Program

3.1. Semantics

Semantics plays a central role in verification since it always serves as a basis to express the properties of interest, that need to be verified, but also additional properties, required to prove the properties of interest, or which may make the design of static analysis easier.

For instance, if we aim for a static analysis that should prove the absence of runtime error in some class of programs, the concrete semantics should define properly what error states and non error states are, and how program executions step from a state to the next one. In the case of a language like C, this includes the behavior of floating point operations as defined in the IEEE 754 standard. When considering parallel programs, this includes a model of the scheduler, and a formalization of the memory model.

In addition to the properties that are required to express the proof of the property of interest, it may also be desirable that semantics describe program behaviors in a finer manner, so as to make static analyses easier to design. For instance, it is well known that, when a state property (such as the absence of runtime error) is valid, it can be established using only a state invariant (i.e., an invariant that ignores the order in which states are visited during program executions). Yet searching for trace invariants (i.e., that take into account some properties of program execution history) may make the static analysis significantly easier, as it will allow it to make finer case splits, directed by the history of program executions. To allow for such powerful static analyses, we often resort to a *non standard semantics*, which incorporates properties that would normally be left out of the concrete semantics.

3.2. Abstract interpretation and static analysis

Once a reference semantics has been fixed and a property of interest has been formalized, the definition of a static analysis requires the choice of an *abstraction*. The abstraction ties a set of *abstract predicates* to the concrete ones, which they denote. This relation is often expressed with a *concretization function* that maps each abstract element to the concrete property it stands for. Obviously, a well chosen abstraction should allow expressing the property of interest, as well as all the intermediate properties that are required in order to prove it (otherwise, the analysis would have no chance to achieve a successful verification). It should also lend itself to an efficient implementation, with efficient data-structures and algorithms for the representation and the manipulation of abstract predicates. A great number of abstractions have been proposed for all kinds of concrete data types, yet the search for new abstractions is a very important topic in static analysis, so as to target novel kinds of properties, to design more efficient or more precise static analyses.

Once an abstraction is chosen, a set of *sound abstract transformers* can be derived from the concrete semantics and that account for individual program steps, in the abstract level and without forgetting any concrete behavior. A static analysis follows as a result of this step by step approximation of the concrete semantics, when the abstract transformers are all computable. This process defines an *abstract interpretation* [13]. The case of loops requires a bit more work as the concrete semantics typically relies on a fixpoint that may not be computable in finitely many iterations. To achieve a terminating analysis we then use *widening operators* [13], which over-approximates the concrete union and ensure termination.

A static analysis defined that way always terminates and produces sound over-approximations of the programs behaviors. Yet, these results may not be precise enough for verification. This is where the art of static analysis design comes into play through, among others:

- the use of more precise, yet still efficient enough abstract domains;
- the combination of application specific abstract domains;
- the careful choice of abstract transformers and widening operators.

3.3. Applications of the notion of abstraction in semantics

In the previous subsections, we sketched the steps in the design of a static analyzer to infer some family of properties, which should be implementable, and efficient enough to succeed in verifying non trivial systems.

Yet, the same principles can also be applied successfully to other goals. In particular, the abstract interpretation framework should be viewed a very general tool to *compare different semantics*, not necessarily with the goal of deriving a static analyzer. Such comparisons may be used in order to prove two semantics equivalent (i.e., one is an abstraction of the other and vice versa), or that a first semantics is strictly more expressive than another one (i.e., the latter can be viewed an abstraction of the former, where the abstraction actually makes some information redundant, which cannot be recovered). A classical example of such comparison is the classification of semantics of transition systems [12], which provides a better understanding of program semantics in general. For instance, this approach can be applied to get a better understanding of the semantics of a programming language, but also to select which concrete semantics should be used as a foundation for a static analysis, or to prove the correctness of a program transformation, compilation or optimization.

3.4. The analysis of biological models

One of our application domains, the analysis of biological models, is not a classical target of static analysis because it aims at analyzing models instead of programs. Yet, the analysis of biological models is closely intertwined with the other application fields of our group. Firstly, abstract interpretation provides a formal understanding of the abstraction process which is inherent to the modeling process. Abstract interpretation is also used to better understand the systematic approaches which are used in the systems biology field to capture the properties of models, until getting formal, fully automatic, and scalable methods. Secondly, abstract interpretation is used to offer various semantics with different grains of abstraction, and, thus, new methods to apprehend the overall behavior of the models. Conversely, some of the methods and abstractions which are developed for biological models are inspired by the analysis of concurrent systems and by security analysis. Lastly, the analysis of biological models raises issues about differential systems, stochastic systems, and hybrid systems. Any breakthrough in these directions will likely be very important to address the important challenge of the certification of critical systems in interaction with their physical environment.

AOSTE Project-Team

3. Research Program

3.1. Models of Computation and Communication (MoCCs)

Participants: Julien Deantoni, Robert de Simone, Frédéric Mallet, Dumitru Potop Butucaru.

Esterel, SyncCharts, synchronous formalisms, Process Networks, Marked Graphs, Kahn networks, compilation, synthesis, formal verification, optimization, allocation, refinement, scheduling

Formal Models of Computation form the basis of our approach to Embedded System Design. Because of the growing importance of communication handling, it is now associated with the name, MoCC in short. The appeal of MoCCs comes from the fact that they combine features of mathematical models (formal analysis, transformation, and verification) with these of executable specifications (close to code level, simulation, and implementation). Examples of MoCCs in our case are mainly synchronous reactive formalisms and dataflow process networks. Various extensions or specific restrictions enforce respectively greater expressivity or more focused decidable analysis results.

DataFlow Process Networks and Synchronous Reactive Languages such as ESTEREL/SYNCCHARTS and SIGNAL/POLYCHRONY [54], [55], [49], [15], [4], [13] share one main characteristics: they are specified in a self-timed or loosely timed fashion, in the asynchronous data-flow style. But formal criteria in their semantics ensure that, under good correctness conditions, a sound synchronous interpretation can be provided, in which all treatments (computations, signaling communications) are precisely temporally mapped. This is refered to as clock calculus in synchronous reactive systems, and leads to a large body of theoretical studies and deep results in the case of DataFlow Process Networks [50], [48] (consider SDF balance equations for instance [56]).

As a result, explicit schedules become an important ingredient of design, which ultimately can be considered and handled by the designer him/herself. In practice such schedules are sought to optimize other parts of the design, mainly buffering queues: production and consumption of data can be regulated in their relative speeds. This was specially taken into account in the recent theories of Latency-Insensitive Design [51], or N-synchronous processes [52], with some of our contributions [6].

Explicit schedule patterns should be pictured in the framework of low-power distributed mapping of embedded applications onto manycore architectures, where they could play an important role as theoretical formal models on which to compute and optimize allocations and performances. We describe below two lines of research in this direction. Striking in these techniques is the fact that they include time and timing as integral parts of early functional design. But this original time is logical, multiform, and only partially ordering the various functional computations and communications. This approach was radically generalized in our team to a methodology for logical time based design, described next (see 3.2).

3.1.1. K-periodic static scheduling and routing in Process Networks

In the recent years we focused on the algorithm treatments of ultimately k-periodic schedule regimes, which are the class of schedules obtained by many of the theories described above. An important breakthrough occurred when realizing that the type of ultimatelly periodic binary words that were used for reporting *static scheduling* results could also be employed to record a completely distinct notion of ultimately k-periodic route switching patterns, and furthermore that commonalities of representation could ease combine them together. A new model, by the name of K-periodical Routed marked Graphs (KRG) was introduced, and extensively studied for algebraic and algorithmic properties [5].

The computations of optimized static schedules and other optimal buffering configurations in the context of latency-insensitive design led to the K-Passa software tool development (now terminated)

3.1.2. Endochrony and GALS implementation of conflict-free polychronous programs

The possibility of exploring various schedulings for a given application comes from the fact that some behaviors are truly concurrent, and mutually *conflict-free* (so they can be executed independently, with any choice of ordering). Discovering potential asynchronous inside synchronous reactive specifications then becomes something highly desirable. It can benefit to potential distributed implementation, where signal communications are restricted to a minimum, as they usually incur loss in performance and higher power consumption. This general line of research has come to be known as Endochrony, with some of our contributions [11].

3.2. Logical Time in Model-Driven Embedded System Design

Participants: Julien Deantoni, Frédéric Mallet, Marie Agnes Peraldi Frati, Robert de Simone.

Starting from specific needs and opportunities for formal design of embedded systems as learned from our work on MoCCs (see 3.1), we developed a Logical Time Model as part of the official OMG UML profile MARTE for Modeling and Analysis of Real-Time Embedded systems. With this model is associated a Clock Constraint Specification Language (CCSL), which allows to provide loose or strict logical time constraints between design ingredients, be them computations, communications, or any kind of events whose repetitions can be conceived as generating a logical conceptual clock (or activation condition). The definition of CCSL is provided in [1].

Our vision is that many (if not all) of the timing constraints generally expressed as physical prescriptions in real-time embedded design (such as periodicity, sporadicity) could be expressed in a logical setting, while actually many physical timing values are still unknown or unspecified at this stage. On the other hand, our logical view may express much more, such as loosely stated timing relations based on partial orderings or partial constraints.

So far we have used CCSL to express important phenonema as present in several formalisms: AADL (used in avionics domain), EAST-ADL2 (proposed for the AutoSar automotive electronic design approach), IP-Xact (for System-on-Chip (*SoC*) design). The difference here comes from the fact that these formalisms were formerly describing such issues in informal terms, while CCSL provides a dedicated formal mathematical notation. Close connections with synchronous and polychronous languages, especially Signal, were also established; so was the ability of CCSL to model dataflow process network static scheduling.

In principle the MARTE profile and its Logical Time Model can be used with any UML editor supporting profiles. It has also evolved to become a Domain-Specific Language, independent of UML. It is connected to the CAPELLA environment, and the PAPYRUS open-source editor. We developed under Eclipse the TIMESQUARE solver and emulator for CCSL constraints (see 5.6), with its own graphical interface, as a stand-alone software module, again now coupled with MARTE and Papyrus, but also as part of the GeMoC studio environment developed in the GeMoC ANR project.

The MARTE profile and its Logical Time Model can be used with any UML editor supporting profiles but evolved to become a DSL independant of UML. We developed as a set of eclipse plugins the TIMESQUARE tool to edit and simulate CCSL specifications. TimeSquare has been coupled with various tools like Papyrus or Capella and is now part of the concurent solver integrated in the GEMOC studio.

While CCSL constraints may be introduced as part of the intended functionality, some may also be extracted from requirements imposed either from real-time user demands, or from the resource limitations and features from the intended execution platform. Sophisticated detailed descriptions of platform architectures are allowed using MARTE, as well as formal allocations of application operations (computations and communications) onto platform resources (processors and interconnects). This is of course of great value at a time where embedded architectures are becoming more and more heterogeneous and parallel or distributed, so that application mapping in terms of spatial allocation and temporal scheduling becomes harder and harder. This approach is extensively supported by the MARTE profile and its various models. As such it originates from the Application-Architecture-Adequation (AAA) methodology, first proposed by Yves Sorel, member of Aoste. AAA aims at specific distributed real-time algorithmic methods, described next in 3.3 .

Of course, while logical time in design is promoted here, and our works show how many current notions used in real-time and embedded systems synthesis can naturally be phrased in this model, there will be in the end a phase of validation of the logical time assumptions (as is the case in synchronous circuits and SoC design with timing closure issues). This validation is usually conducted from Worst-Case Execution Time (WCET) analysis on individual components, which are then used in further analysis techniques to establish the validity of logical time assumptions (as partial constraints) asserted during the design.

3.3. The AAA (Algorithm-Architecture Adequation) methodology and Real-Time Scheduling

Participants: Liliana Cucu, Laurent George, Dumitru Potop Butucaru, Yves Sorel.

Note: The AAA methodology and the SynDEx environment are fully described at http://www.syndex.org/, together with relevant publications.

3.3.1. Algorithm-Architecture Adequation

The AAA methodology relies on distributed real-time scheduling and relevant optimization to connect an Algorithm/Application model to an Architectural one. We now describe its premises and benefits.

The Algorithm model is an extension of the well known data-flow model from Dennis [53]. It is a directed acyclic hyper-graph (DAG) that we call “conditioned factorized data dependence graph”, whose vertices are “operations” and hyper-edges are directed “data or control dependences” between operations. The data dependences define a partial order on the operations execution. The basic data-flow model was extended in three directions: first infinite (resp. finite) repetition of a sub-graph pattern in order to specify the reactive aspect of real-time systems (resp. in order to specify the finite repetition of a sub-graph consuming different data similar to a loop in imperative languages), second “state” when data dependences are necessary between different infinite repetitions of the sub-graph pattern introducing cycles which must be avoided by introducing specific vertices called “delays” (similar to z^{-n} in automatic control), third “conditioning” of an operation by a control dependence similar to conditional control structure in imperative languages, allowing the execution of alternative subgraphs. Delays combined with conditioning allow the programmer to specify automata necessary for describing “mode changes”.

The Architecture model is a directed graph, whose vertices are of two types: “processor” (one sequencer of operations and possibly several sequencers of communications) and “medium” (support of communications), and whose edges are directed connections.

The resulting implementation model [9] is obtained by an external compositional law, for which the architecture graph operates on the algorithm graph. Thus, the result of such compositional law is an algorithm graph, "architecture-aware", corresponding to refinements of the initial algorithm graph, by computing spatial (distribution) and timing (scheduling) allocations of the operations onto the architecture graph resources. In that context "Adequation" refers to some search amongst the solution space of resulting algorithm graphs, labelled by timing characteristics, for one algorithm graph which verifies timing constraints and optimizes some criteria, usually the total execution time and the number of computing resources (but other criteria may exist). The next section describes distributed real-time schedulability analysis and optimization techniques for that purpose.

3.3.2. Distributed Real-Time Scheduling and Optimization

We address two main issues: uniprocessor and multiprocessor real-time scheduling where constraints must mandatorily be met, otherwise dramatic consequences may occur (hard real-time) and where resources must be minimized because of embedded features.

In the case of uniprocessor real-time scheduling, besides the classical deadline constraint, often equal to a period, we take into consideration dependences beetween tasks and several, latencies. The latter are complex related “end-to-end” constraints. Dealing with multiple real-time constraints raises the complexity of the scheduling problems. Moreover, because the preemption leads, at least, to a waste of resources due to its approximation in the WCET (Worst Execution Time) of every task, as proposed by Liu and Leyland [57], we first studied non-preemtive real-time scheduling with dependences, periodicities, and latencies constraints. Although a bad approximation of the preemption cost, may have dramatic consequences on real-time scheduling, there are only few researches on this topic. We have been investigating preemptive real-time scheduling since few years, and we focus on the exact cost of the preemption. We have integrated this cost in the schedulability conditions that we propose, and in the corresponding scheduling algorithms. More generally, we are interested in integrating in the schedulability analyses the cost of the RTOS (Real-Time Operating System), for which the cost of preemption is the most difficult part because it varies according to the instance (job) of each task.

In the case of multiprocessor real-time scheduling, we chose at the beginning the partitioned approach, rather than the global approach, since the latter allows task migrations whose cost is prohibitive for current commercial processors. The partitioned approach enables us to reuse the results obtained in the uniprocessor case in order to derive solutions for the multiprocessor case. We consider also the semi-partitioned approach which allows only some migrations in order to minimize the overhead they involve. In addition to satisfy the multiple real-time constraints mentioned in the uniprocessor case, we have to minimize the total execution time (makespan) since we deal with automatic control applications involving feedback loops. Furthermore, the domain of embedded systems leads to solving minimization resources problems. Since these optimization problems are NP-hard we develop exact algorithms (B & B, B & C) which are optimal for simple problems, and heuristics which are sub-optimal for realistic problems corresponding to industrial needs. Long time ago we proposed a very fast “greedy” heuristics [8] whose results were regularly improved, and extended with local neighborhood heuristics, or used as initial solutions for metaheuristics.

In addition to the spatial dimension (distributed) of the real-time scheduling problem, other important dimensions are the type of communication mechanisms (shared memory vs. message passing), or the source of control and synchronization (event-driven vs. time-triggered). We explore real-time scheduling on architectures corresponding to all combinations of the above dimensions. This is of particular impact in application domains such as automotive and avionics (see 4.3).

The arrival of complex hardware responding to the increasing demand for computing power in next generation systems exacerbates the limitations of the current worst-case real-time reasoning. Our solution to overcome these limitations is based on the fact that worst-case situations may have a extremely low probability of appearance within one hour of functioning (10^{-45}), compared to the certification requirements for instance (10^{-9} for the highest level of certification in avionics). Thus we model and analyze the real-time systems using probabilistic models and we propose results that are fundamental for the probabilistic worst-case reasoning over a given time window.

ARIC Project-Team

3. Research Program

3.1. Efficient approximation methods

3.1.1. Computer algebra generation of certified approximations

We plan to focus on the generation of certified and efficient approximations for solutions of linear differential equations. These functions cover many classical mathematical functions and many more can be built by combining them. One classical target area is the numerical evaluation of elementary or special functions. This is currently performed by code specifically handcrafted for each function. The computation of approximations and the error analysis are major steps of this process that we want to automate, in order to reduce the probability of errors, to allow one to implement “rare functions”, to quickly adapt a function library to a new context: new processor, new requirements – either in terms of speed or accuracy.

In order to significantly extend the current range of functions under consideration, several methods originating from approximation theory have to be considered (divergent asymptotic expansions; Chebyshev or generalized Fourier expansions; Padé approximants; fixed point iterations for integral operators). We have done preliminary work on some of them. Our plan is to revisit them all from the points of view of effectivity, computational complexity (exploiting linear differential equations to obtain efficient algorithms), as well as in their ability to produce provable error bounds. This work is to constitute a major progress towards the automatic generation of code for moderate or arbitrary precision evaluation with good efficiency. Other useful, if not critical, applications are certified quadrature, the determination of certified trajectories of spatial objects and many more important questions in optimal control theory.

3.1.2. Digital Signal Processing

As computer arithmeticians, a wide and important target for us is the design of efficient and certified linear filters in digital signal processing (DSP). Actually, following the advent of MATLAB as the major tool for filter design, the DSP experts now systematically delegate to MATLAB all the part of the design related to numerical issues. And yet, various key MATLAB routines are neither optimized, nor certified. Therefore, there is a lot of room for enhancing numerous DSP numerical implementations and there exist several promising approaches to do so.

The main challenge that we want to address over the next period is the development and the implementation of optimal methods for rounding the coefficients involved in the design of the filter. If done in a naive way, this rounding may lead to a significant loss of performance. We will study in particular FIR and IIR filters.

3.1.3. Table Maker’s Dilemma (TMD)

There is a clear demand for hardest-to-round cases, and several computer manufacturers recently contacted us to obtain new cases. These hardest-to-round cases are a precious help for building libraries of correctly rounded mathematical functions. The current code, based on Lefèvre’s algorithm, will be rewritten and formal proofs will be done.

We plan to use uniform polynomial approximation and diophantine techniques in order to tackle the case of the IEEE quad precision, and analytic number theory techniques (exponential sums estimates) for counting the hardest-to-round cases.

3.2. Lattices: algorithms and cryptology

Lattice-based cryptography (LBC) is an utterly promising, attractive (and competitive) research ground in cryptography, thanks to a combination of unmatched properties:

- **Improved performance.** LBC primitives have low asymptotic costs, but remain cumbersome in practice (e.g., for parameters achieving security against computations of up to 2100 bit operations). To address this limitation, a whole branch of LBC has evolved where security relies on the restriction of lattice problems to a family of more structured lattices called *ideal lattices*. Primitives based on such lattices can have quasi-optimal costs (i.e., quasi-constant amortized complexities), outperforming all contemporary primitives. This asymptotic performance sometimes translates into practice, as exemplified by NTRUEncrypt.
- **Improved security.** First, lattice problems seem to remain hard even for quantum computers. Moreover, the security of most of LBC holds under the assumption that standard lattice problems are hard in the worst case. Oppositely, contemporary cryptography assumes that specific problems are hard with high probability, for some precise input distributions. Many of these problems were artificially introduced for serving as a security foundation of new primitives.
- **Improved flexibility.** The master primitives (encryption, signature) can all be realized based on worst-case (ideal) lattice assumptions. More evolved primitives such as ID-based encryption (where the public key of a recipient can be publicly derived from its identity) and group signatures, that were the playing-ground of pairing-based cryptography (a subfield of elliptic curve cryptography), can also be realized in the LBC framework, although less efficiently and with restricted security properties. More intriguingly, lattices have enabled long-wished-for primitives. The most notable example is homomorphic encryption, enabling computations on encrypted data. It is the appropriate tool to securely outsource computations, and will help overcome the privacy concerns that are slowing down the rise of the cloud.

We work on three directions, detailed now.

3.2.1. Lattice algorithms

All known lattice reduction algorithms follow the same design principle: perform a sequence of small elementary steps transforming a current basis of the input lattice, where these steps are driven by the Gram-Schmidt orthogonalisation of the current basis.

In the short term, we will fully exploit this paradigm, and hopefully lower the cost of reduction algorithms with respect to the lattice dimension. We aim at asymptotically fast algorithms with complexity bounds closer to those of basic and normal form problems (matrix multiplication, Hermite normal form). In the same vein, we plan to investigate the parallelism potential of these algorithms.

Our long term goal is to go beyond the current design paradigm, to reach better trade-offs between run-time and shortness of the output bases. To reach this objective, we first plan to strengthen our understanding of the interplay between lattice reduction and numerical linear algebra (how far can we push the idea of working on approximations of a basis?), to assess the necessity of using the Gram-Schmidt orthogonalisation (e.g., to obtain a weakening of LLL-reduction that would work up to some stage, and save computations), and to determine whether working on generating sets can lead to more efficient algorithms than manipulating bases. We will also study algorithms for finding shortest non-zero vectors in lattices, and in particular look for quantum accelerations.

We will implement and distribute all algorithmic improvements, e.g., within the fplll library. We are interested in high performance lattice reduction computations (see application domains below), in particular in connection with/continuation of the HPAC ANR project (algebraic computing and high performance consortium).

3.2.2. Lattice-based cryptography

Our long term goal is to demonstrate the superiority of lattice-based cryptography over contemporary public-key cryptographic approaches. For this, we will 1- Strengthen its security foundations, 2- Drastically improve the performance of its primitives, and 3- Show that lattices allow to devise advanced and elaborate primitives.

The practical security foundations will be strengthened by the improved understanding of the limits of lattice reduction algorithms (see above). On the theoretical side, we plan to attack two major open problems: Are ideal lattices (lattices corresponding to ideals in rings of integers of number fields) computationally as hard to handle as arbitrary lattices? What is the quantum hardness of lattice problems?

Lattice-based primitives involve two types of operations: sampling from discrete Gaussian distributions (with lattice supports), and arithmetic in polynomial rings such as $(\mathbb{Z}/q\mathbb{Z})[x]/(x^n+1)$ with n a power of 2. When such polynomials are used (which is the case in all primitives that have the potential to be practical), then the underlying algorithmic problem that is assumed hard involves ideal lattices. This is why it is crucial to precisely understand the hardness of lattice problems for this family. We will work on improving both types of operations, both in software and in hardware, concentrating on values of q and n providing security. As these problems are very arithmetic in nature, this will naturally be a source of collaboration with the other themes of the AriC team.

Our main objective in terms of cryptographic functionality will be to determine the extent to which lattices can help securing cloud services. For example, is there a way for users to delegate computations on their outsourced dataset while minimizing what the server eventually learns about their data? Can servers compute on encrypted data in an efficiently verifiable manner? Can users retrieve their files and query remote databases anonymously provided they hold appropriate credentials? Lattice-based cryptography is the only approach so far that has allowed to make progress into those directions. We will investigate the practicality of the current constructions, the extension of their properties, and the design of more powerful primitives, such as functional encryption (allowing the recipient to learn only a function of the plaintext message). To achieve these goals, we will in particular focus on cryptographic multilinear maps.

This research axis of AriC is gaining strength thanks to the recruitment of Benoit Libert. We will be particularly interested in the practical and operational impacts, and for this reason we envision a collaboration with an industrial partner.

3.2.3. Application domains

- Diophantine equations. Lattice reduction algorithms can be used to solve diophantine equations, and in particular to find simultaneous rational approximations to real numbers. We plan to investigate the interplay between this algorithmic task, the task of finding integer relations between real numbers, and lattice reduction. A related question is to devise LLL-reduction algorithms that exploit specific shapes of input bases. This will be done within the ANR DynA3S project.
- Communications. We will continue our collaboration with Cong Ling (Imperial College) on the use of lattices in communications. We plan to work on the wiretap channel over a fading channel (modeling cell phone communications in a fast moving environment). The current approaches rely on ideal lattices, and we hope to be able to find new approaches thanks to our expertise on them due to their use in lattice-based cryptography. We will also tackle the problem of sampling vectors from Gaussian distributions with lattice support, for a very small standard deviation parameter. This would significantly improve current schemes for communication schemes based on lattices, as well as several cryptographic primitives.
- Cryptanalysis of variants of RSA. Lattices have been used extensively to break variants of the RSA encryption scheme, via Coppersmith's method to find small roots of polynomials. We plan to work with Nadia Heninger (U. of Pennsylvania) on improving these attacks, to make them more practical. This is an excellent test case for testing the practicality of LLL-type algorithm. Nadia Heninger has a strong experience in large scale cryptanalysis based on Coppersmith's method (http://smartfacts.cr.yp.to/)

3.3. Algebraic computing and high performance kernels

The main theme here is the study of fundamental operations ("kernels") on a hierarchy of symbolic or numeric data types spanning integers, floating-point numbers, polynomials, power series, as well as matrices of all these. Fundamental operations include basic arithmetic (e.g., how to multiply or how to invert) common to all such data, as well as more specific ones (change of representation/conversions, GCDs, determinants, etc.). For such operations, which are ubiquitous and at the very core of computing (be it numerical, symbolic, or hybrid numeric-symbolic), our goal is to ensure both high performance and reliability.

3.3.1. Algorithms

On the symbolic side, we will focus on the design and complexity analysis of algorithms for matrices over various domains (fields, polynomials, integers) and possibly with specific properties (structure). So far, our algorithmic improvements for polynomial matrices and structured matrices have been obtained in a rather independent way. Both types are well known to have much in common, but this is sometimes not reflected by the complexities obtained, especially for applications in cryptology and coding theory. Our goal in this area is thus to explore these connections further, to provide a more unified treatment, and eventually bridge these complexity gaps, A first step towards this goal will be the design of enhanced algorithms for various generalizations of Hermite-Padé approximation; in the context of list decoding, this should in particular make it possible to match or even improve over the structured-matrix approach, which is so far the fastest known.

On the other hand we will focus on the design of algorithms for certified computing. We will study the use of various representations, such as mid-rad for classical interval arithmetic, or affine arithmetic. We will explore the impact of precision tuning in intermediate computations, possibly dynamically, on the accuracy of the results (e.g. for iterative refinement and Newton iterations). We will continue to revisit and improve the classical error bounds of numerical linear algebra in the light of the subtleties of IEEE floating-point arithmetic.

Our goals in linear algebra and lattice basis reduction that have been detailed above in Section 3.2 will be achieved in the light of a hybrid symbolic-numeric approach.

3.3.2. Computer arithmetic

Our work on certified computing and especially on the analysis of algorithms in floating-point arithmetic leads us to manipulate floating-point data in their greatest generality, that is, as symbolic expressions in the base and the precision. Our aim here is thus to develop theorems as well as efficient data structures and algorithms for handling such quantities by computer rather than by hand as we do now. The main outcome would be a "symbolic floating-point toolbox" which provides a way to check automatically the certificates of optimality we have obtained on the error bounds of various numerical algorithms.

We will also work on the interplay between floating-point and integer arithmetics. Currently, small numerical kernels like an exponential or a 2×2 determinant are typically written using exclusively one of these two kinds of arithmetic. However, modern processors now have hardware support for both floating-point and integer arithmetics, often with vector (SIMD) extensions, and an important question is how to make the best use of all such capabilities to optimize for both accuracy and efficiency.

A third direction will be to work on algorithms for performing correctly-rounded arithmetic operations in medium precision as efficiently and reliably as possible. Indeed, many numerical problems require higher precision than the conventional floating-point (single, double) formats. One solution is to use multiple precision libraries, such as GNU MPFR, which allow the manipulation of very high precision numbers, but their generality (they are able to handle numbers with millions of digits) is a quite heavy alternative when high performance is needed. Our objective here is thus to design a multiple precision arithmetic library that would allow to tackle problems where a precision of a few hundred bits is sufficient, but which have strong performance requirements. Applications include the process of long-term iteration of chaotic dynamical systems ranging from the classical Henon map to calculations of planetary orbits. The designed algorithms will be formally proved.

Finally, our work on the IEEE 1788 standard leads naturally to the development of associated reference libraries for interval arithmetic. A first direction will be to implement IEEE 1788 interval arithmetic within MPFI, our library for interval arithmetic using the arbitrary precision floating-point arithmetic provided by MPFR: indeed, MPFI has been originally developed with definitions and handling of exceptions which are not compliant with IEEE 1788. Another one will be to provide efficient support for multiple-precision intervals, in mid-rad representation and by developing MPFR-based code-generation tools aimed at handling families of functions.

3.3.3. High-performance algorithms and software

The algorithmic developments for medium precision floating-point arithmetic discussed above will lead to high performance implementations on GPUs. As a follow-up of the HPAC project (which ended in December 2015) we shall pursue the design and implementation of high performance linear algebra primitives and algorithms.

AROMATH Project-Team

3. Research Program

3.1. High order geometric modeling

The accurate description of shapes is a long standing problem in mathematics, with an important impact in many domains, inducing strong interactions between geometry and computation. Developing precise geometric modeling techniques is a critical issue in CAD-CAM. Constructing accurate models, that can be exploited in geometric applications, from digital data produced by cameras, laser scanners, observations or simulations is also a major issue in geometry processing. A main challenge is to construct models that can capture the geometry of complex shapes, using few parameters while being precise.

Our first objective is to develop methods, which are able to describe accurately and in an efficient way, objects or phenomena of geometric nature, using algebraic representations.

The approach followed in CAGD, to describe complex geometry is based on parametric representations called NURBS (Non Uniform Rational B-Spline). The models are constructed by trimming and gluing together high order patches of algebraic surfaces. These models are built from the so-called B-Spline functions that encode a piecewise algebraic function with a prescribed regularity at the seams. Although these models have many advantages and have become the standard for designing nowadays CAD models,they also have important drawbacks. Among them, the difficulty to locally refine a NURBS surface and also the topological rigidity of NURBS patches that imposes to use many such patches with trims for designing complex models, with the consequence of the appearing of cracks at the seams. To overcome these difficulties, an active area of research is to look for new blending functions for the representation of CAD models. Some examples are the so-called T-Splines, LR-Spline blending functions, or hierarchical splines, that have been recently devised in order to perform efficiently local refinement. An important problem is to analyze spline spaces associated to general subdivisions, which is of particular interest in higher order Finite Element Methods. Another challenge in geometric modeling is the efficient representation and/or reconstruction of complex objects, and the description of computational domains in numerical simulation To construct models that can represent efficiently the geometry of complex shapes, we are interested in developing modeling methods, based on alternative constructions such as skeleton-based representations. The change of representation, in particular between parametric and implicit representations, is of particular interest in geometric computations and in its applications in CAGD.

We also plan to investigate adaptive hierarchical techniques, which can locally improve the approximation of a shape or a function. They shall be exploited to transform digital data produced by cameras, laser scanners, observations or simulations into accurate and structured algebraic models.

The precise and efficient representation of shapes also leads to the problem of extracting and exploiting characteristic properties of shapes such as symmetry, which is very frequent in geometry. Reflecting the symmetry of the intended shape in the representation appears as a natural requirement for visual quality, but also as a possible source of sparsity of the representation. Recognizing, encoding and exploiting symmetry requires new paradigms of representation and further algebraic developments. Algebraic foundations for the exploitation of symmetry in the context of non linear differential and polynomial equations are addressed. The intent is to bring this expertise with symmetry to the geometric models and computations developed by AROMATH.

3.2. Robust algebraic-geometric computation

In many problems, digital data are approximated and cannot just be used as if they were exact. In the context of geometric modeling, polynomial equations appear naturally, as a way to describe constraints between the unknown variables of a problem. *An important challenge is to take into account the input error in order to* *develop robust methods for solving these algebraic constraints.* Robustness means that a small perturbation of the input should produce a controlled variation of the output, that is forward stability, when the input-output map is regular. In non-regular cases, robustness also means that the output is an exact solution, or the most coherent solution, of a problem with input data in a given neighborhood, that is backward stability.

Our second long term objective is to develop methods to robustly and efficiently solve algebraic problems that occur in geometric modeling.

Robustness is a major issue in geometric modeling and algebraic computation. Classical methods in computer algebra, based on the paradigm of exact computation, cannot be applied directly in this context. They are not designed for stability against input perturbations. New investigations are needed to develop methods, which integrate this additional dimension of the problem. Several approaches are investigated to tackle these difficulties.

One is based on linearization of algebraic problems based on “elimination of variables” or projection into a space of smaller dimension. Resultant theory provides strong foundation for these methods, connecting the geometric properties of the solutions with explicit linear algebra on polynomial vector spaces, for families of polynomial systems (e.g., homogeneous, multi-homogeneous, sparse). Important progresses have been made in the last two decades to extend this theory to new families of problems with specific geometric properties. Additional advances have been achieved more recently to exploit the syzygies between the input equations. This approach provides matrix based representations, which are particularly powerful for approximate geometric computation on parametrized curves and surfaces. They are tuned to certain classes of problems and an important issue is to detect and analyze degeneracies and to adapt them to these cases.

A more adaptive approach involves linear algebra computation in a hierarchy of polynomial vector spaces. It produces a description of quotient algebra structures, from which the solutions of polynomial systems can be recovered.This family of methods includes Gröbner Basis, which provides general tools for solving polynomial equations. Border Basis is an alternative approach, offering numerically stable methods for solving polynomial equations with approximate coefficients. An important issue is to understand and control the numerical behavior of these methods as well as their complexity and to exploit the structure of the input system.

In order to compute “only” the (real) solutions of a polynomial system in a given domain, duality techniques can also be employed. They consist in analyzing and adding constraints on the space of linear forms which vanish on the polynomial equations. Combined with semi-definite programming techniques, they provide efficient methods to compute the real solutions of algebraic equations or to solve polynomial optimization problems.The main issues are the completness of the approach, their scalability with the degree and dimension and the certification of bounds.

Singular solutions of polynomial systems can be analyzed by computing differentials, which vanish at these points. This leads to efficient deflation techniques, which transform a singular solution of a given problem into a regular solution of the transformed problem. These local methods need to be combined with more global root localisation methods.

Subdivision methods are another type of methods which are interesting for robust geometric computation. They are based on exclusion tests which certify that no solution exits in a domain and inclusion tests, which certify the uniqueness of a solution in a domain. They have shown their strength in addressing many algebraic problems, such as isolating real roots of polynomial equations or computing the topology of algebraic curves and surfaces. The main issues in these approaches is to deal with singularities and degenerate solutions.

CAIRN Project-Team

3. Research Program

3.1. Panorama

The development of complex applications is traditionally split in three stages: a theoretical study of the algorithms, an analysis of the target architecture and the implementation. When facing new emerging applications such as high-performance, low-power and low-cost mobile communication systems or smart sensor-based systems, it is mandatory to strengthen the design flow by a joint study of both algorithmic and architectural issues.

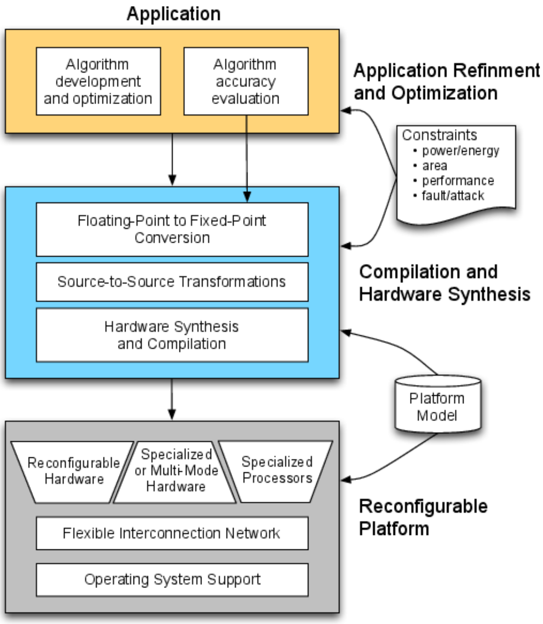

Application
Algorithm development and optimization
Algorithm accuracy evaluation
Application Refinment and Optimization
Constraints
• power/energy
• area
• performance
• fault/attack
Floating-Point to Fixed-Point Conversion
Source-to-Source Transformations
Hardware Synthesis and Compilation
Compilation and Hardware Synthesis
Platform Model
Reconfigurable Hardware
Specialized or Multi-Mode Hardware
Specialized Processors
Flexible Interconnection Network
Operating System Support
Reconfigurable Platform

Figure 1. CAIRN's general design flow and related research themes

Figure 1 shows the global design flow we propose to develop. This flow is organized in levels which refer to our three research themes: application optimization (new algorithms, fixed-point arithmetic, advanced representations of numbers), architecture optimization (reconfigurable and specialized hardware, application-specific processors, arithmetic operators and functions), and stepwise refinement and code generation (code transformations, hardware synthesis, compilation).

In the rest of this part, we briefly describe the challenges concerning **new reconfigurable platforms** in Section 3.2 and the issues on **compiler and synthesis tools** related to these platforms in Section 3.3 .

3.2. Reconfigurable Architecture Design

Nowadays, FPGAs are not only suited for application specific algorithms, but also considered as fully-featured computing platforms, thanks to their ability to accelerate massively parallelizable algorithms much faster than their processor counterparts [84]. They also support to be dynamically reconfigured. At runtime, partially reconfigurable regions of the logic fabric can be reconfigured to implement a different task, which allows for a better resource usage and adaptation to the environment. Dynamically reconfigurable hardware can also cope with hardware errors by relocating some of its functionalities to another, sane, part of the logic fabric. It could also provide support for a multi-tasked computation flow where hardware tasks are loaded on-demand at runtime. Nevertheless, current design flows of FPGA vendors are still limited by the use of one partial bitstream for each reconfigurable region and for each design. These regions are defined at design time and it is not possible to use only one bitstream for multiple reconfigurable regions nor multiple chips. The multiplicity of such bitstreams leads to a significant increase in memory. Recent research has been conducted in the domain of task relocation on a reconfigurable fabric. All of the related work was conducted on architectures from commercial vendors (e.g., Xilinx, Altera) which share the same limitations: the inner details of the bitstream are not publicly known, which limits applicability of the techniques. To circumvent this issue, most dynamic reconfiguration techniques are either generating multiple bitstreams for each location [66] or implementing an online filter to relocate the tasks [78]. Both of these techniques still suffer from memory footprint and from the online complexity of task relocation.

Increasing the level and grain of reconfiguration is a solution to counterbalance the FPGA penalties. Coarse-grained reconfigurable architectures (CGRA) provide operator-level configurable functional blocks and word-level datapaths [85], [72], [83]. Compared to FPGA, they benefit from a massive reduction in configuration memory and configuration delay, as well as for routing and placement complexity. This in turns results in an improvement in the computation volume over energy cost ratio, although with a loss of flexibility compared to bit-level operations. Such constraints have been taken into account in the design of DART[10], Adres [81] or polymorphous computing fabrics[12]. These works have led to commercial products such as the PACT/XPP [65] or Montium from Recore systems, without however a real commercial success yet. Emerging platforms like Xilinx/Zynq or Intel/Altera are about to change the game.

In the context of emerging heterogenous multicore architecture, CAIRN advocates for associating general-purpose processors (GPP), flexible network-on-chip and coarse-grain or fine-grain dynamically reconfigurable accelerators. We leverage our skills on microarchitecture, reconfigurable computing, arithmetic, and low-power design, to discover and design such architectures with a focus on: -reduced energy per operation, -improved application performance through acceleration, - hardware flexibility and self-adaptive behavior, -tolerance to faults, computing errors, and process variation, - protections against side channel attacks, - limited silicon area overhead.

3.3. Compilation and Synthesis for Reconfigurable Platforms

In spite of their advantages, reconfigurable architectures, and more generally hardware accelerators, lack efficient and standardized compilation and design tools. As of today, this still makes the technology impractical for large-scale industrial use. Generating and optimizing the mapping from high-level specifications to reconfigurable hardware platforms are therefore key research issues, which have received considerable interest over the last years [70], [86], [82], [80], [79]. In the meantime, the complexity (and heterogeneity) of these platforms has also been increasing quite significantly, with complex heterogeneous multi-cores architectures becoming a *de facto* standard. As a consequence, the focus of designers is now geared toward optimizing overall system-level performance and efficiency [77]. Here again, existing tools are not well suited, as they fail at providing an unified programming view of the programmable and/or reconfigurable components implemented on the platform.

In this context, we have been pursuing our efforts to propose tools whose design principles are based on a tight coupling between the compiler and the target hardware architectures. We build on the expertise of the team members in High Level Synthesis (HLS) [6], ASIP optimizing compilers [13] and automatic parallelization for massively parallel specialized circuits [2]. We first study how to increase the efficiency of standard programmable processors by extending their instruction set to speed-up compute intensive kernels. Our focus is on efficient and exact algorithms for the identification, selection and scheduling of such instructions [7]. We address compilation challenges by borrowing techniques from high-level synthesis, optimizing compilers and automatic parallelization, especially when dealing with nested loop kernels. In addition, and independently of the scientific challenges mentioned above, proposing such flows also poses significant software engineering issues. As a consequence, we also study how leading edge software engineering techniques (Model Driven Engineering) can help the Computer Aided Design (CAD) and optimizing compiler communities prototyping new research ideas [14], [5], [3].

Efficient implementation of multimedia and signal processing applications (in software for DSP cores or as special-purpose hardware) often requires, for reasons related to cost, power consumption or silicon area constraints, the use of fixed-point arithmetic, whereas the algorithms are usually specified in floating-point arithmetic. Unfortunately, fixed-point conversion is very challenging and time-consuming, typically demanding up to 50% of the total design or implementation time. Thus, tools are required to automate this conversion. For hardware or software implementation, the aim is to optimize the fixed-point specification. The implementation cost is minimized under a numerical accuracy or an application performance constraint. For DSP-software implementation, methodologies have been proposed [8] to achieve fixed-point conversion. For hardware implementation, the best results are obtained when the word-length optimization process is coupled with the high-level synthesis [73]. Evaluating the effects of finite precision is one of the major and often the most time consuming step while performing fixed-point refinement. Indeed, in the word-length optimization process, the numerical accuracy is evaluated as soon as a new word-length is tested, thus, several times per iteration of the optimization process. Classical approaches are based on fixed-point simulations [74]. Leading to long evaluation times, they can hardly be used to explore the design space. Therefore, our aim is to propose closed-form expressions of errors due to fixed-point approximations that are used by a fast analytical framework for accuracy evaluation [11].

CAMUS Team

3. Research Program

3.1. Research Directions

The various objectives we are expecting to reach are directly related to the search of adequacy between the sofware and the new multicore processors evolution. They also correspond to the main research directions suggested by Hall, Padua and Pingali in [24]. Performance, correction and productivity must be the users' perceived effects. They will be the consequences of research works dealing with the following issues:

- Issue 1: Static Parallelization and Optimization
- Issue 2: Profiling and Execution Behavior Modeling
- Issue 3: Dynamic Program Parallelization and Optimization, Virtual Machine
- Issue 4: Proof of Program Transformations for Multicores

Efficient and correct applications development for multicore processors needs stepping in every application development phase, from the initial conception to the final run.

Upstream, all potential parallelism of the application has to be exhibited. Here static analysis and transformation approaches (issue 1) must be processed, resulting in a *multi-parallel* intermediate code advising the running virtual machine about all the parallelism that can be taken advantage of. However the compiler does not have much knowledge about the execution environment. It obviously knows the instruction set, it can be aware of the number of available cores, but it does not know the effective available resources at any time during the execution (memory, number of free cores, etc.).

That is the reason why a "virtual machine" mechanism will have to adapt the application to the resources (issue 3). Moreover the compiler will be able to take advantage only of a part of the parallelism induced by the application. Indeed some program information (variables values, accessed memory adresses, etc.) being available only at runtime, another part of the available parallelism will have to be generated on-the-fly during the execution, here also, thanks to a dynamic mechanism.

This on-the-fly parallelism extraction will be performed using speculative behavior models (issue 2), such models allowing to generate speculative parallel code (issue 3). Between our behavior modeling objectives, we can add the behavior monitoring, or profiling, of a program version. Indeed current and future architectures complexity avoids assuming an optimal behavior regarding a given program version. A monitoring process will allow to select on-the-fly the best parallelization.

These different parallelizing steps are schematized on figure 1 .

Our project lies on the conception of a production chain for efficient execution of an application on a multicore architecture. Each link of this chain has to be formally verified in order to ensure correction as well as efficiency. More precisely, it has to be ensured that the compiler produces a correct intermediate code, and that the virtual machine actually performs the parallel execution semantically equivalent to the source code: every transformation applied to the application, either statically by the compiler or dynamically by the virtual machine, must preserve the initial semantics. They must be proved formally (issue 4).

In the following, those different issues are detailed while forming our global and long term vision of what has to be done.

3.2. Static Parallelization and Optimization

Participants: Vincent Loechner, Philippe Clauss, Éric Violard, Cédric Bastoul, Arthur Charguéraud.

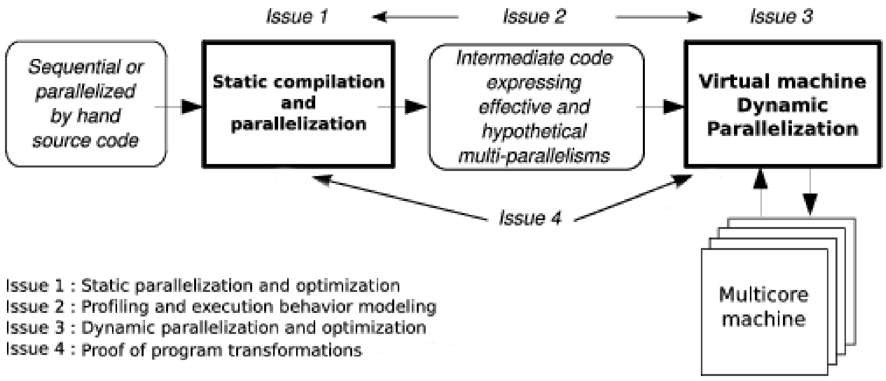

Issue 1
Issue 2
Issue 3
Sequential or parallelized by hand source code
Static compilation and parallelization
Intermediate code expressing effective and hypothetical multi-parallelisms
Virtual machine Dynamic Parallelization
Issue 4
Multicore machine
Issue 1 : Static parallelization and optimization
Issue 2 : Profiling and execution behavior modeling
Issue 3 : Dynamic parallelization and optimization
Issue 4 : Proof of program transformations

Figure 1. Automatic parallelizing steps for multicore architectures

Static optimizations, from source code at compile time, benefit from two decades of research in automatic parallelization: many works address the parallelization of loop nests accessing multi-dimensional arrays, and these works are now mature enough to generate efficient parallel code [23]. Low-level optimizations, in the assembly code generated by the compiler, have also been extensively dealt for single-core and require few adaptations to support multicore architectures. Concerning multicore specific parallelization, we propose to explore two research directions to take full advantage of these architectures: adapting parallelization to multicore architecture and expressing many potential parallelisms.

3.3. Profiling and Execution Behavior Modeling

Participants: Alain Ketterlin, Philippe Clauss, Manuel Selva.

The increasing complexity of programs and hardware architectures makes it ever harder to characterize beforehand a given program's run time behavior. The sophistication of current compilers and the variety of transformations they are able to apply cannot hide their intrinsic limitations. As new abstractions like transactional memories appear, the dynamic behavior of a program strongly conditions its observed performance. All these reasons explain why empirical studies of sequential and parallel program executions have been considered increasingly relevant. Such studies aim at characterizing various facets of one or several program runs, *e.g.*, memory behavior, execution phases, etc. In some cases, such studies characterize more the compiler than the program itself. These works are of tremendous importance to highlight all aspects that escape static analysis, even though their results may have a narrow scope, due to the possible incompleteness of their input data sets.

3.4. Dynamic Parallelization and Optimization, Virtual Machine

Participants: Manuel Selva, Juan Manuel Martinez Caamaño, Luis Esteban Campostrini, Artiom Baloian, Mariem Saied, Daniel Salas, Philippe Clauss, Jens Gustedt, Vincent Loechner, Alain Ketterlin.

This link in the programming chain has become essential with the advent of the new multicore architectures. Still being considered as secondary with mono-core architectures, dynamic analysis and optimization are now one of the keys for controling those new mechanisms complexity. From now on, performed instructions are not only dedicated to the application functionalities, but also to its control and its transformation, and so in its own interest. Behaving like a computer virus, such a process should rather be qualified as a “vitamin”. It perfectly knows the current characteristics of the execution environment and owns some qualitative information thanks to a behavior modeling process (issue 2). It appends a significant part of optimizing ability compared to a static compiler, while observing live resources availability evolution.

3.5. Proof of Program Transformations for Multicores

Participants: Éric Violard, Alain Ketterlin, Julien Narboux, Nicolas Magaud, Arthur Charguéraud.

Our main objective consists in certifying the critical modules of our optimization tools (the compiler and the virtual machine). First we will prove the main loop transformation algorithms which constitute the core of our system.

The optimization process can be separated into two stages: the transformations consisting in optimizing the sequential code and in exhibiting parallelism, and those consisting in optimizing the parallel code itself. The first category of optimizations can be proved within a sequential semantics. For the other optimizations, we need to work within a concurrent semantics. We expect the first stage of optimizations to produce data-race free code. For the second stage of optimizations, we will first assume that the input code is data-race free. We will prove those transformations using Appel's concurrent separation logic [25]. Proving transformations involving program which are not data-race free will constitute a longer term research goal.

CARAMBA Project-Team

3. Research Program

3.1. The Extended Family of the Number Field Sieve

The Number Field Sieve (NFS) has been the leading algorithm for factoring integers for more than 20 years, and its variants have been used to set records for discrete logarithms in finite fields. It is reasonable to understand NFS as a framework that can be used to solve various sorts of problems. Factoring integers and computing discrete logarithms are the most prominent for the cryptographic observer, but the same framework can also be applied to the computation of class groups.

The state of the art with NFS is built from numerous improvements of its inner steps. In terms of algorithmic improvements, the recent research activity on the NFS family has been rather intense. Several new algorithms have been discovered in over the 2014–2016 period, and their practical reach has been demonstrated by actual experiments.

The algorithmic contributions of the CARAMBA members to NFS would hardly be possible without access to a dependable software implementation. To this end, members of the CARAMBA team have been developing the Cado-NFS software suite since 2007. Cado-NFS is now the most widely visible open source implementation of NFS, and is a crucial platform for developing prototype implementations for new ideas for the many sub-algorithms of NFS. Cado-NFS is free software (LGPL) and follows an open development model, with publicly accessible development repository and regular software releases. Competing free software implementations exist, such as `msieve`, developed by J. Papadopoulos. In Lausanne, T. Kleinjung develops his own code base, which is unfortunately not public.

The workplan of CARAMBA on the topic of the Number Field Sieve algorithm and its cousins includes the following aspects:

- Pursue the work on NFS, which entails in particular making it ready to tackle larger challenges. Several of the important computational steps of NFS that are currently identified as stumbling blocks will require algorithmic advances and implementation improvements. We will illustrate the importance of this work by computational records.
- Work on the specific aspects of the computation of discrete logarithms in finite fields.
- As a side topic, the application of the broad methodology of NFS to the treatment of “ideal lattices” and their use in cryptographic proposals based on Euclidean lattices is also relevant.

3.2. Algebraic Curves in Cryptology

The challenges associated to algebraic curves in cryptology are diverse, because of the variety of mathematical objects to be considered. These challenges are also connected to each other. On the cryptographic side, efficiency matters. As of 2016, the most widely used set of elliptic curves, the so-called NIST curves, are in the process of being replaced by a new set of candidate elliptic curves for future standardization. This is the topic of RFC 7748 [34].

On the cryptanalytic side, the discrete logarithm problem on (Jacobians of) curves has resisted all attempts for many years. Among the currently active topics, the decomposition algorithms raise interesting problems related to polynomial system solving, as do attempts to solve the discrete logarithm problem on curves defined over binary fields. In particular, while it is generally accepted that the so-called Koblitz curves (base field extensions of curves defined over $\mathrm{GF}(2)$) are likely to be a weak class among the various curve choices, no concrete attack supports this claim fully.

The research objectives of CARAMBA on the topic of algebraic curves for cryptology are as follows:

- Work on the practical realization of some of the rich mathematical theory behind algebraic curves. In particular, some of the fundamental mathematical objects have potentially important connections to the broad topic of cryptology: Abel-Jacobi map, Theta functions, computation of isogenies, computation of endomorphisms, complex multiplication.
- Improve the point counting algorithms so as to be able to tackle larger problems. This includes significant work connected to polynomial systems.
- Seek improvements on the computation of discrete logarithms on curves, including by identifying weak instances of this problem.

3.3. Computer Arithmetic

Computer arithmetic is part of the common background of all team members, and is naturally ubiquitous in the two previous application domains mentioned. However involved the mathematical objects considered may be, dealing with them first requires to master more basic objects: integers, finite fields, polynomials, and real and complex floating-point numbers. Libraries such as GNU MP, GNU MPFR, GNU MPC do an excellent job for these, both for small and large sizes (we rarely, if ever, focus on small-precision floating-point data, which explains our lack of mention of libraries relevant to it).

Most of our involvement in subjects related to computer arithmetic is to be understood in connection to our applications to the Number Field Sieve and to abelian varieties. As such, much of the research work we envision will appear as side-effects of developments in these contexts. On the topic of arithmetic work *per se*:

- We will seek algorithmic and practical improvements to the most basic algorithms. That includes for example the study of advances algorithms for integer multiplication, and their practical reach.
- We will continue to work on the arithmetic libraries in which we have crucial involvement, such as GNU MPFR, GNU MPC, GF2X, MPFQ, and also GMP-ECM.

3.4. Polynomial Systems

Systems of polynomial equations have been part of the cryptographic landscape for quite some time, with applications to the cryptanalysis of block and stream ciphers, as well as multivariate cryptographic primitives.

Polynomial systems arising from cryptology are usually not generic, in the sense that they have some distinct structural properties, such as symmetries, or bi-linearity for example. During the last decades, several results have shown that identifying and exploiting these structures can lead to dedicated Gröbner bases algorithms that can achieve large speedups compared to generic implementations [27], [26].

Solving polynomial systems is well done by existing software, and duplicating this effort is not relevant. However we develop test-bed open-source software for ideas relevant to the specific polynomial systems that arise in the context of our applications. The TinyGB software, that we describe further in 6.3 , is our platform to test new ideas.

We aim to work on the topic of polynomial system solving in connection with our involvement in the aforementioned topics.

- We have high expertise on Elliptic Curve Discrete Logarithm Problem on small characteristic finite fields, because it also involves highly structured polynomial systems. While so far we have not contributed to this hot topic, this could of course change in the future.
- Recent hirings (Minier) are likely to lead the team to study particular polynomial systems in context which are more related to symmetric key cryptography.
- More centered on polynomial systems *per se*, we will mainly pursue the study of the specificities of the polynomial systems that are strongly linked to our targeted applications, and for which we have significant expertise [27], [26]. We also want to see these recent results provide practical benefits compared to existing software, in particular for systems relevant for cryptanalysis.

CARTE Team

3. Research Program

3.1. Computer Virology

From a historical point of view, the first official virus appeared in 1983 on Vax-PDP 11. At the same time, a series of papers was published which always remains a reference in computer virology: Thompson [71], Cohen [42] and Adleman [29]. The literature which explains and discusses practical issues is quite extensive [46], [48]. However, there are only a few theoretical/scientific studies, which attempt to give a model of computer viruses.

A virus is essentially a self-replicating program inside an adversary environment. Self-replication has a solid background based on works on fixed point in λ-calculus and on studies of von Neumann [76]. More precisely we establish in [38] that Kleene's second recursion theorem [60] is the cornerstone from which viruses and infection scenarios can be defined and classified. The bottom line of a virus behavior is

1. a virus infects programs by modifying them,
2. a virus copies itself and can mutate,
3. it spreads throughout a system.

The above scientific foundation justifies our position to use the word virus as a generic word for self-replicating malwares. There is yet a difference. A malware has a payload, and virus may not have one. For example, a worm is an autonomous self-replicating malware and so falls into our definition. In fact, the current malware taxonomy (virus, worms, trojans, ...) is unclear and subject to debate.

3.2. Computation over continuous structures

Classical recursion theory deals with computability over discrete structures (natural numbers, finite symbolic words). There is a growing community of researchers working on the extension of this theory to continuous structures arising in mathematics. One goal is to give foundations of numerical analysis, by studying the limitations of machines in terms of computability or complexity, when computing with real numbers. Classical questions are : if a function $f:\mathbb{R}\to\mathbb{R}$ is computable in some sense, are its roots computable? in which time? Another goal is to investigate the possibility of designing new computation paradigms, transcending the usual discrete-time, discrete-space computer model initiated by the Turing machine that is at the base of modern computers.

While the notion of a computable function over discrete data is captured by the model of Turing machines, the situation is more delicate when the data are continuous, and several non-equivalent models exist. In this case, let us mention computable analysis, which relates computability to topology [45], [74]; the Blum-Shub-Smale model (BSS), where the real numbers are treated as elementary entities [37]; the General Purpose Analog Computer (GPAC) introduced by Shannon [69]with continuous time.

3.3. Rewriting

The rewriting paradigm is now widely used for specifying, modelizing, programming and proving. It allows one to easily express deduction systems in a declarative way, and to express complex relations on infinite sets of states in a finite way, provided they are countable. Programming languages and environments with a rewriting based semantics have been developed ; see ASF+SDF [39], MAUDE [41], and TOM [66].

For basic rewriting, many techniques have been developed to prove properties of rewrite systems like confluence, completeness, consistency or various notions of termination. Proof methods have also been proposed for extensions of rewriting such as equational extensions, consisting of rewriting modulo a set of axioms, conditional extensions where rules are applied under certain conditions only, typed extensions, where rules are applied only if there is a type correspondence between the rule and the term to be rewritten, and constrained extensions, where rules are enriched by formulas to be satisfied [32], [44], [70].

An interesting aspect of the rewriting paradigm is that it allows automatable or semi-automatable correctness proofs for systems or programs: the properties of rewriting systems as those cited above are translatable to the deduction systems or programs they formalize and the proof techniques may directly apply to them.

Another interesting aspect is that it allows characteristics or properties of the modeled systems to be expressed as equational theorems, often automatically provable using the rewriting mechanism itself or induction techniques based on completion [43]. Note that the rewriting and the completion mechanisms also enable transformation and simplification of formal systems or programs.

Applications of rewriting-based proofs to computer security are various. Approaches using rule-based specifications have recently been proposed for detection of computer viruses [72], [73]. For several years, in our team, we have also been working in this direction. We already proposed an approach using rewriting techniques to abstract program behaviors for detecting suspicious or malicious programs [34], [35].

CASCADE Project-Team

3. Research Program

3.1. Randomness in Cryptography

Randomness is a key ingredient for cryptography. Random bits are necessary not only for generating cryptographic keys, but are also often an important part of cryptographic algorithms. In some cases, probabilistic protocols make it possible to perform tasks that are impossible deterministically. In other cases, probabilistic algorithms are faster, more space efficient or simpler than known deterministic algorithms. Cryptographers usually assume that parties have access to perfect randomness but in practice this assumption is often violated and a large body of research is concerned with obtaining such a sequence of random or pseudorandom bits.

One of the project-team research goals is to get a better understanding of the interplay between randomness and cryptography and to study the security of various cryptographic protocols at different levels (information-theoretic and computational security, number-theoretic assumptions, design and provable security of new and existing constructions).

Cryptographic literature usually pays no attention to the fact that in practice randomness is quite difficult to generate and that it should be considered as a resource like space and time. Moreover since the perfect randomness abstraction is not physically realizable, it is interesting to determine whether imperfect randomness is “good enough” for certain cryptographic algorithms and to design algorithms that are robust with respect to deviations of the random sources from true randomness.

The power of randomness in computation is a central problem in complexity theory and in cryptography. Cryptographers should definitely take these considerations into account when proposing new cryptographic schemes: there exist computational tasks that we only know how to perform efficiently using randomness but conversely it is sometimes possible to remove randomness from probabilistic algorithms to obtain efficient deterministic counterparts. Since these constructions may hinder the security of cryptographic schemes, it is of high interest to study the efficiency/security tradeoff provided by randomness in cryptography.

Quite often in practice, the random bits in cryptographic protocols are generated by a pseudorandom number generation process. When this is done, the security of the scheme of course depends in a crucial way on the quality of the random bits produced by the generator. Despite the importance, many protocols used in practice often leave unspecified what pseudorandom number generation to use. It is well-known that pseudorandom generators exist if and only if one-way functions exist and there exist efficient constructions based on various number-theoretic assumptions. Unfortunately, these constructions are too inefficient and many protocols used in practice rely on “ad-hoc” constructions. It is therefore interesting to propose more efficient constructions, to analyze the security of existing ones and of specific cryptographic constructions that use weak pseudorandom number generators.

The project-team undertakes research in these three aspects. The approach adopted is both theoretical and practical, since we provide security results in a mathematical frameworks (information theoretic or computational) with the aim to design protocols among the most efficient known.

3.2. Lattice Cryptography

The security of almost all public-key cryptographic protocols in use today relies on the presumed hardness of problems from number theory such as factoring and discrete log. This is somewhat problematic because these problems have very similar underlying structure, and its unforeseen exploit can render all currently used public key cryptography insecure. This structure was in fact exploited by Shor to construct efficient quantum algorithms that break all hardness assumptions from number theory that are currently in use. And so naturally, an important area of research is to build provably-secure protocols based on mathematical problems that are unrelated to factoring and discrete log. One of the most promising directions in this line of research is using lattice problems as a source of computational hardness —in particular since they also offer features that other alternative public-key cryptosystems (such as MQ-based, code-based or hash-based schemes) cannot provide.

At its very core, secure communication rests on two foundations: authenticity and secrecy. Authenticity assures the communicating parties that they are indeed communicating with each other and not with some potentially malicious outside party. Secrecy is necessary so that no one except the intended recipient of a message is able to deduce anything about its contents.

Lattice cryptography might find applications towards constructing practical schemes for resolving essential cryptographic problems —in particular, guaranteeing authenticity. On this front, our team is actively involved in pursuing the following two objectives:

1. Construct, implement, and standardize a practical public key digital signature scheme that is secure against quantum adversaries.
2. Construct, implement, and standardize a symmetric key authentication scheme that is secure against side channel attacks and is more efficient than the basic scheme using AES with masking.

Despite the great progress in constructing fairly practical lattice-based encryption and signature schemes, efficiency still remains a very large obstacle for advanced lattice primitives. While constructions of identity-based encryption schemes, group signature schemes, functional encryption schemes, and even fully-homomorphic encryption schemes are known, the implementations of these schemes are extremely inefficient.

Fully Homomorphic Encryption (FHE) is a very active research area. Let us just give one example illustrating the usefulness of computing on encrypted data: Consider an on-line patent database on which firms perform complex novelty queries before filing patents. With current technologies, the database owner might analyze the queries, infer the invention and apply for a patent before the genuine inventor. While such frauds were not reported so far, similar incidents happen during domain name registration. Several websites propose "registration services" preceded by "availability searches". These queries trigger the automated registration of the searched domain names which are then proposed for sale. Algorithms allowing arbitrary computations without disclosing their inputs (and/or their results) are hence of immediate usefulness.

In 2009, IBM announced the discovery of a FHE scheme by Craig Gentry. The security of this algorithm relies on worst-case problems over ideal lattices and on the hardness of the sparse subset sum problem. Gentry's construction is an ingenious combination of two ideas: a somewhat homomorphic scheme (capable of supporting many "logical or" operations but very few "ands") and a procedure that refreshes the homomorphically processed ciphertexts. Gentry's main conceptual achievement is a "bootstrapping" process in which the somewhat homomorphic scheme evaluates its own decryption circuit (self-reference) to refresh (recrypt) ciphertexts.

Unfortunately, it is safe to surmise that if the state of affairs remains as it is in the present, then despite all the theoretical efforts that went into their constructions, these schemes will never be used in practical applications.

Our team is looking at the foundations of these primitives with the hope of achieving a breakthrough that will allow them to be practical in the near future.

3.3. Security amidst Concurrency on the Internet

Cryptographic protocols that are secure when executed in isolation, can be completely insecure when multiple such instances are executed concurrently (as is unavoidable on the Internet) or when used as a part of a larger protocol. For instance, a man-in-the-middle attacker participating in two simultaneous executions of a cryptographic protocol might use messages from one of the executions in order to compromise the security of the second – Lowe's attack on the Needham-Schroeder authentication protocol and Bleichenbacher's attack on SSL work this way. Our research addresses security amidst concurrent executions in secure computation and key exchange protocols.

Secure computation allows several mutually distrustful parties to collaboratively compute a public function of their inputs, while providing the same security guarantees as if a trusted party had performed the computation. Potential applications for secure computation include anonymous voting as well as privacy-preserving auctions and data-mining. Our recent contributions on this topic include

1. new protocols for secure computation in a model where each party interacts only once, with a single centralized server; this model captures communication patterns that arise in many practical settings, such as that of Internet users on a website,

2. and efficient constructions of universally composable commitments and oblivious transfer protocols, which are the main building blocks for general secure computation.

In key exchange protocols, we are actively involved in designing new password-authenticated key exchange protocols, as well as the analysis of the widely-used SSL/TLS protocols.

3.4. Electronic Currencies

Electronic cash (e-cash) was first proposed in the 1980s but despite extensive research it has never been deployed on a large scale. Other means of digital payments have instead largely replaced cash and other "analog" payments. Common to all digital payments offered by banks and other payment providers is that they do not respect the citizens' right to privacy, which for legitimate purchases and moderate sums also includes their right of anonymous payments.

Recently the rise of so-called decentralized currencies, such as Bitcoin and the numerous "alt-coins" inspired by it, have established a third way of payments in addition to physical cash, which offers privacy, and card and other electronic payments, which are traceable by its providers. The continuous growth of popularity and usage of this new kind of currencies, also called "cryptocurrencies" as their security and stability crucially relies on the use of cryptography, have triggered a renewed interest in cryptographic e-cash.

Our group investigates "centralized" e-cash, which respects the current economic model where money is issued by (central) banks, as opposed to cryptocurrencies, which use money distribution to incentivize widespread participation in the system, required for stability. Of particular interest among centralized e-cash schemes is transferable e-cash, which allows users to transfer coins between each other without any interaction with a third party. Currently all efficient e-cash schemes require coins to be deposited at the bank once received; they are thus not transferable. Our goal is to propose efficient transferable e-cash schemes.

Another direction concerns cryptocurrencies whose adoption is continuously growing so that now even central banks, like the Swedish *Riksbank*, are considering issuing their own currency as a cryptocurrency. While systems like Bitcoin are perceived as offering anonymous payments, a line of research has shown that this is not the case. One of the major research challenges in this area is thus to devise schemes that offer an anonymity level comparable to that of physical cash. The currently proposed schemes either lack formal security analyses or they are inefficient due to the heavy-duty cryptography used. Our group works towards practical cryptocurrencies with formally analyzed privacy guarantees.

CELTIQUE Project-Team (section vide)

COMETE Project-Team

3. Research Program

3.1. Probability and information theory

Participants: Konstantinos Chatzikokolakis, Catuscia Palamidessi, Ehab Elsalamouny, Tymofii Prokopenko, Joris Lamare.

Much of the research of Comète focuses on security and privacy. In particular, we are interested in the problem of the leakage of secret information through public observables.

Ideally we would like systems to be completely secure, but in practice this goal is often impossible to achieve. Therefore, we need to reason about the amount of information leaked, and the utility that it can have for the adversary, i.e. the probability that the adversary is able to exploit such information.

The recent tendency is to use an information theoretic approach to model the problem and define the leakage in a quantitative way. The idea is to consider the system as an information-theoretic *channel*. The input represents the secret, the output represents the observable, and the correlation between the input and output (*mutual information*) represents the information leakage.

Information theory depends on the notion of entropy as a measure of uncertainty. From the security point of view, this measure corresponds to a particular model of attack and a particular way of estimating the security threat (vulnerability of the secret). Most of the proposals in the literature use Shannon entropy, which is the most established notion of entropy in information theory. We, however, consider also other notions, in particular Rényi min-entropy, which seems to be more appropriate for security in common scenarios like one-try attacks.

3.2. Expressiveness of Concurrent Formalisms

Participants: Catuscia Palamidessi, Frank Valencia.

We study computational models and languages for distributed, probabilistic and mobile systems, with a particular attention to expressiveness issues. We aim at developing criteria to assess the expressive power of a model or formalism in a distributed setting, to compare existing models and formalisms, and to define new ones according to an intended level of expressiveness, also taking into account the issue of (efficient) implementability.

3.3. Concurrent constraint programming

Participants: Michell Guzman, Yamil Salim Perchy, Frank Valencia.

Concurrent constraint programming (ccp) is a well established process calculus for modeling systems where agents interact by posting and asking information in a store, much like in users interact in *social networks*. This information is represented as first-order logic formulae, called constraints, on the shared variables of the system (e.g., $X > 42$). The most distinctive and appealing feature of ccp is perhaps that it unifies in a single formalism the operational view of processes based upon process calculi with a declarative one based upon first-order logic. It also has an elegant denotational semantics that interprets processes as closure operators (over the set of constraints ordered by entailment). In other words, any ccp process can be seen as an idempotent, increasing, and monotonic function from stores to stores. Consequently, ccp processes can be viewed as: computing agents, formulae in the underlying logic, and closure operators. This allows ccp to benefit from the large body of techniques of process calculi, logic and domain theory.

Our research in ccp develops along the following two lines:

1. **(a)** The study of a bisimulation semantics for ccp. The advantage of bisimulation, over other kinds of semantics, is that it can be efficiently verified.
2. **(b)** The extension of ccp with constructs to capture emergent systems such as those in social networks and cloud computing.

3.4. Model checking

Participants: Konstantinos Chatzikokolakis, Catuscia Palamidessi.

Model checking addresses the problem of establishing whether a given specification satisfies a certain property. We are interested in developing model-checking techniques for verifying concurrent systems of the kind explained above. In particular, we focus on security and privacy, i.e., on the problem of proving that a given system satisfies the intended security or privacy properties. Since the properties we are interested in have a probabilistic nature, we use probabilistic automata to model the protocols. A challenging problem is represented by the fact that the interplay between nondeterminism and probability, which in security presents subtleties that cannot be handled with the traditional notion of a scheduler,

COMPSYS Team

3. Research Program

3.1. Architecture and Compilation Trends

The embedded system design community is facing two challenges:

- The complexity of embedded applications is increasing at a rapid rate.
- The needed increase in processing power is no longer obtained by increases in the clock frequency, but by increased parallelism.

While, in the past, each type of embedded application was implemented in a separate appliance, the present tendency is toward a universal hand-held object, which must serve as a cell-phone, as a personal digital assistant, as a game console, as a camera, as a Web access point, and much more. One may say that embedded applications are of the same level of complexity as those running on a PC, but they must use a more constrained platform in terms of processing power, memory size, and energy consumption. Furthermore, most of them depend on international standards (e.g., in the field of radio digital communication), which are evolving rapidly. Lastly, since ease of use is at a premium for portable devices, these applications must be integrated seamlessly to a degree that is unheard of in standard computers.

All of this dictates that modern embedded systems retain some form of programmability. For increased designer productivity and reduced time-to-market, programming must be done in some high-level language, with appropriate tools for compilation, run-time support, and debugging. This does not mean however that all embedded systems (or all of an embedded system) must be processor based. Another solution is the use of field programmable gate arrays (FPGA), which may be programmed at a much finer grain than a processor, although the process of FPGA "programming" is less well understood than software generation. Processors are better than application-specific circuits at handling complicated control and unexpected events. On the other hand, FPGAs may be tailored to just meet the needs of their application, resulting in better energy and silicon area usage. It is expected that most embedded systems will use a combination of general-purpose processors, specific processors like DSPs, and FPGA accelerators (or even low-power GPUs). Such a combination DSP+FPGA is already present in recent versions of the Atom Intel processor.

As a consequence, parallel programming, which has long been confined to the high-performance community, must become the common place rather than the exception. In the same way that sequential programming moved from assembly code to high-level languages at the price of a slight loss in performance, parallel programming must move from low-level tools, like OpenMP or even MPI, to higher-level programming environments. While fully-automatic parallelization is a Holy Grail that will probably never be reached in our lifetimes, it will remain as a component in a comprehensive environment, including general-purpose parallel programming languages, domain-specific parallelizers, parallel libraries and run-time systems, back-end compilation, dynamic parallelization. The landscape of embedded systems is indeed very diverse and many design flows and code optimization techniques must be considered. For example, embedded processors (micro-controllers, DSP, VLIW) require powerful back-end optimizations that can take into account hardware specificities, such as special instructions and particular organizations of registers and memories. FPGA and hardware accelerators, to be used as small components in a larger embedded platform, require "hardware compilation", i.e., design flows and code generation mechanisms to generate non-programmable circuits. For the design of a complete system-on-chip platform, architecture models, simulators, debuggers are required. The same is true for multicores of any kind, GPGPU ("general-purpose" graphical processing units), CGRA (coarse-grain reconfigurable architectures), which require specific methodologies and optimizations, although all these techniques converge or have connections. In other words, embedded systems need all usual aspects of the process that transforms some specification down to an executable, software or hardware. In this wide range of topics, Compsys concentrated on the code optimizations aspects (and the associated analysis) in this transformation chain, restricting to compilation (transforming a program to a program) for embedded processors and programmable accelerators, and to high-level synthesis (transforming a program into a circuit description) for FPGAs.

Actually, it is not a surprise to see compilation and high-level synthesis getting closer (in the last 10 years now). Now that high-level synthesis has grown up sufficiently to be able to rely on place-and-route tools, or even to synthesize C-like languages, standard techniques for back-end code generation (register allocation, instruction selection, instruction scheduling, software pipelining) are used in HLS tools. At the higher level, programming languages for programmable parallel platforms share many aspects with high-level specification languages for HLS, for example the description and manipulations of nested loops, or the model of computation/communication (e.g., Kahn process networks and its many "streaming" variants). In all aspects, the frontier between software and hardware is vanishing. For example, in terms of architecture, customized processors (with processor extensions as first proposed by Tensilica) share features with both general-purpose processors and hardware accelerators. FPGAs are both hardware and software as they are fed with "programs" representing their hardware configurations.

In other words, this convergence in code optimizations explains why Compsys studied both program compilation and high-level synthesis, and at both front-end and back-end levels, the first one acting more at the granularity of memories, transfers, and multiple cores, the second one more at the granularity of registers, system calls, and single core. Both levels must be considered as they interact with each other. Front-end optimizations must be aware of what back-end optimizations will do, as single core performance remain the basis for good parallel performances. Some front-end optimizations even act directly on back-end features, for example register tiling considered as a source-level transformation. Also, from a conceptual point of view, the polyhedral techniques developed by Compsys are actually the symbolic front-end counterpart, for structured loops, of back-end analysis and optimizations of unstructured programs (through control-flow graphs), such as dependence analysis, scheduling, lifetime analysis, register allocation, etc. A strength of Compsys was to juggle with both aspects, the first one based on graph theory with SSA-type optimizations, the other on polyhedra representing loops, and to exploit the correspondence between both. This has still to be exploited, for applying polyhedral techniques to more irregular programs. Besides, Compsys had a tradition of building free software tools for linear programming and optimization in general, as needed for our research.

3.1.1. Compilation and Languages Issues in the Context of Embedded Processors, "Embedded Systems", and Programmable Accelerators

Compilation is an old activity, in particular back-end code optimizations. The development of embedded systems was one of the reasons for the revival of compilation activities as a research topic. Applications for embedded computing systems generate complex programs and need more and more processing power. This evolution is driven, among others, by the increasing impact of digital television, the first instances of UMTS networks, and the increasing size of digital supports, like recordable DVD, and even Internet applications. Furthermore, standards are evolving very rapidly (see for instance the successive versions of MPEG). As a consequence, the industry has focused on programmable structures, whose flexibility more than compensates for their larger size and power consumption. The appliance provider has a choice between hard-wired structures (Asic), special-purpose processors (Asip), (quasi) general-purpose processors (DSP for multimedia applications), and now hardware accelerators (dedicated platforms – such as those developed by Thales or the CEA –, or more general-purpose accelerators such as GPUs or even multicores, even if these are closer to small HPC platforms than truly embedded systems). Our cooperation with STMicroelectronics, until 2012, focused on investigating the compilation for specialized processors, such as the ST100 (DSP processor) and the ST200 (VLIW DSP processor) family. Even for this restricted class of processors, the diversity is large, and the potential for instruction level parallelism (SIMD, MMX), the limited number of registers and the small size of the memory, the use of direct-mapped instruction caches, of predication, generated many open problems. Our goal was to contribute to their understanding and their solutions.

An important concept to cope with the diversity of platforms is the concept of *virtualization*, which is a key for more portability, more simplicity, more reliability, and of course more security. This concept – implemented at low level through binary translation and just-in-time (JIT) compilation [0] – consists in hiding the architecture-dependent features as long as possible during the compilation process. It has been used for a while for servers such as HotSpot, a bit more recently for workstations, and now for embedded computing. The same needs drive the development of intermediate languages such as OpenCL to, not necessarily hide, but at least make more uniform, the different facets of the underlying architectures. The challenge is then to design and compile high-productivity and high-performance languages [0] (coping with parallelism and heterogeneity) that can be ported to such intermediate languages, or to architecture-dependent runtime systems. The offloading of computation kernels, through source-to-source compilation, targeting back-end C dialects, has the same goals: to automate application porting to the variety of accelerators.

For JIT compilation, the compactness of the information representation, and thus its pertinence, is an important criterion for such late compilation phases. Indeed, the intermediate representation (IR) is evolving not only from a target-independent description to a target-dependent one, but also from a situation where the compilation time is almost unlimited (cross-compilation) to one where any type of resource is limited. This is one of the reasons why static single assignment (SSA), a sparse compact representation of liveness information, became popular in embedded compilation. If time constraints are common to all JIT compilers (not only for embedded computing), the benefit of using SSA is also in terms of its good ratio pertinence/storage of information. It also enables to simplify algorithms, which is also important for increasing the reliability of the compiler. In this context, our aim has been, in particular, to develop exact or heuristic solutions to *combinatorial* problems that arise in compilation for VLIW and DSP processors, and to integrate these methods into industrial compilers for DSP processors (mainly ST100, ST200, Strong ARM). Such combinatorial problems can be found in register allocation, opcode selection, code placement, when removing the SSA multiplexer functions (known as ϕ functions). These optimizations are usually done in the last phases of the compiler, using an assembly-level intermediate representation. As mentioned in Sections 2.3 and 2.4 , we made a lot of progress in this area in our past collaborations with STMicroelectronics (see also previous activity reports). Through the Sceptre and Mediacom projects, we first revisited, in the light of SSA, some code optimizations in an aggressive context, to develop better strategies, without eliminating too quickly solutions that may have been considered as too expensive in the past. Then we exploited the new concepts introduced in the aggressive context to design better algorithms in a JIT context, focusing on the speed of algorithms and their memory footprint, without compromising too much on the quality of the generated code.

Our recent research directions were more focused on programmable accelerators, such as GPU and multicores, but still considering *static* compilation and without forgetting the link between high-level (in general at source-code level) and low-level (i.e., at assembly-code level) optimizations. They concerned program analysis (of both sequential and parallel specifications), program optimizations (for memory hierarchies, parallelism, streaming, etc.), and also the link with applications, and between compilers and users (programmers). Polyhedral techniques play an important role in these directions, even if control-flow-based techniques remain in the background and may come back at any time in the foreground. This is also the case for high-level synthesis, as exposed in the next section.

3.1.2. Context of High-Level Synthesis and FPGA Platforms

High-level synthesis has become a necessity, mainly because the exponential increase in the number of gates per chip far outstrips the productivity of human designers. Besides, applications that need hardware accelerators usually belong to domains, like telecommunications and game platforms, where fast turn-around and time-to-market minimization are paramount. When Compsys started, we were convinced that our expertise in compilation and automatic parallelization could contribute to the development of the needed tools.

[0] *Aggressive compilation* consists in allowing more time to implement more complete and costly solutions: compilation time is less relevant than execution time, size, and energy consumption of the produced code, which can have a critical impact on the cost and quality of the final product. The application is usually cross-compiled, i.e., compiled on a powerful platform distinct from the target processor. *Just-in-time compilation*, on the other hand, corresponds to compiling applets on demand on the target processor. The code can be uploaded or sold separately on a flash memory. Compilation is performed at load time and even dynamically during execution. The optimization heuristics, constrained by time and limited resources, are far from being aggressive. They must be fast but smart enough.

[0] For examples of such languages, see the keynotes event we organized in 2013: http://labexcompilation.ens-lyon.fr/hpc-languages.

Today, synthesis tools for FPGAs or ASICs come in many shapes. At the lowest level, there are proprietary Boolean, layout, and place-and-route tools, whose input is a VHDL or Verilog specification at the structural or register-transfer level (RTL). Direct use of these tools is difficult, for several reasons:

- A structural description is completely different from an usual algorithmic language description, as it is written in term of interconnected basic operators. One may say that it has a spatial orientation, in place of the familiar temporal orientation of algorithmic languages.
- The basic operators are extracted from a library, which poses problems of selection, similar to the instruction selection problem in ordinary compilation.
- Since there is no accepted standard for VHDL synthesis, each tool has its own idiosyncrasies and reports its results in a different format. This makes it difficult to build portable HLS tools.
- HLS tools have trouble handling loops. This is particularly true for logic synthesis systems, where loops are systematically unrolled (or considered as sequential) before synthesis. An efficient treatment of loops needs the polyhedral model. This is where past results from the automatic parallelization community are useful.
- More generally, a VHDL specification is too low level to allow the designer to perform, easily, higher-level code optimizations, especially on multi-dimensional loops and arrays, which are of paramount importance to exploit parallelism, pipelining, and perform communication and memory optimizations.

Some intermediate tools were proposed that generate VHDL from a specification in restricted C, both in academia (such as SPARK, Gaut, UGH, CloogVHDL), and in industry (such as C2H, CatapultC, Pico-Express, Vivado HLS). All these tools use only the most elementary form of parallelization, equivalent to instruction-level parallelism in ordinary compilers, with some limited form of block pipelining, and communication through FIFOs. Targeting one of these tools for low-level code generation, while we concentrate on exploiting loop parallelism, might be a more fruitful approach than directly generating VHDL. However, it may be that the restrictions they impose preclude efficient use of the underlying hardware. Our first experiments with these HLS tools reveal two important issues. First, they are, of course, limited to certain types of input programs so as to make their design flows successful, even if, over the years, they become more and more mature. But it remains a painful and tricky task for the user to transform the program so that it fits these constraints and to tune it to get good results. Automatic or semi-automatic program transformations can help the user achieve this task. Second, users, even expert users, have only a very limited understanding of what back-end compilers do and why they do not lead to the expected results. An effort must be done to analyze the different design flows of HLS tools, to explain what to expect from them, and how to use them to get a good quality of results. Our first goal was thus to develop high-level techniques that, used in front of existing HLS tools, improve their utilization. This should also give us directions on how to modify them or to design new tools from scratch.

More generally, HLS has to be considered as a more global parallelization process. So far, no HLS tools is capable of generating designs with communicating *parallel* accelerators, even if, in theory, at least for the scheduling part, a tool such as Pico-Express could have such capabilities. The reason is that it is, for example, very hard to automatically design parallel memories and to decide the distribution of array elements in memory banks to get the desired performances with parallel accesses. Also, how to express communicating processes at the language level? How to express constraints, pipeline behavior, communication media, etc.? To better exploit parallelism, a first solution is to extend the source language with parallel constructs, as in all derivations of the Kahn process networks model, including communicating regular processes (CRP). The other solution is a form of automatic parallelization. However, classical methods, which are mostly based on scheduling, need to be revisited, to pay more attention to locality, process streaming, and low-level pipelining, which are of paramount importance in hardware. Besides, classical methods mostly rely on the runtime system to tailor the parallelism degree to the available resources. Obviously, there is no runtime system in hardware. The real challenge is thus to invent new scheduling algorithms that take resource, locality, and pipelining into account, and then to infer the necessary hardware from the schedule. This is probably possible only for programs that fit into the polyhedral model, or in an incrementally-extended model.

Our research activities on polyhedral code analysis and optimizations directly targeted these HLS challenges. But they are not limited to the automatic generation of hardware as can be seen from our different contributions on X10, OpenStream, parametric tiling, etc. The same underlying concepts also arise when optimizing codes for GPUs and multicores. In this context of polyhedral analysis and optimizations, we focused on three aspects:

- developing high-level transformations, especially for loops and memory/communication optimizations, that can be used in front of HLS tools so as to improve their use, as well as for hardware accelerators;
- developing concepts and techniques in a more global view of high-level synthesis and high-level parallel programming, starting from specification languages down to hardware implementation;
- developing more general code analysis so as to extract more information from codes as well as to extend the programs that can be handled.

3.2. Code Analysis, Code Transformations, Code Optimizations

Embedded systems, as we recalled earlier, generated new problems in code analysis and optimization both for optimizing embedded software (compilation) and hardware (HLS). We now give a bit more details on some general challenges for program analysis, optimizations, and transformations, induced by this context, and on our methodology, in particular our development and use of polyhedral optimizations and its extensions.

3.2.1. Processes, Scheduling, Mapping, Communications, etc.

Before mapping an application to an architecture, one has to decide which execution model is targeted and where to intervene in the design flow. Then one has to solve scheduling, placement, and memory management problems. These three aspects should be handled as a whole, but present state of the art dictates that they be treated separately. One of our aims was to develop more comprehensive solutions. The last task is code generation, both for the processing elements and the interfaces processors/accelerators.

There are basically two execution models for embedded systems: one is the classical accelerator model, in which data is deposited in the memory of the accelerator, which then does its job, and returns the results. In the streaming model, computations are done on the fly, as data items flow from an input channel to the output. Here, the data are never stored in (addressable) memory. Other models are special cases, or sometimes compositions of the basic models. For instance, a systolic array follows the streaming model, and sometimes extends it to higher dimensions. Software radio modems follow the streaming model in the large, and the accelerator model in detail. The use of first-in first-out queues (FIFO) in hardware design is an application of the streaming model. Experience shows that designs based on the streaming model are more efficient that those based on memory, for such applications. One of the point to be investigated is whether it is general enough to handle arbitrary (regular) programs. The answer is probably negative. One possible implementation of the streaming model is as a network of communicating processes either as Kahn process networks (FIFO based) or as our more recent model of communicating regular processes (memory based, such as CRP mentioned hereafter). It is an interesting fact that several researchers have investigated the translation from process networks [12] and to process networks [20], [21]. Streaming languages such as StreamIt and OpenStream are also interesting solutions to explore.

Kahn process networks (KPN) were introduced 30 years ago as a notation for representing parallel programs. Such a network is built from processes that communicate via perfect FIFO channels. Because the channel histories are deterministic, one can define a semantics and talk meaningfully about the equivalence of two implementations. As a bonus, the dataflow diagrams used by signal processing specialists can be translated on-the-fly into process networks. The problem with KPNs is that they rely on an asynchronous execution model, while VLIW processors and FPGAs are synchronous or partially synchronous. Thus, there is a need for a tool for synchronizing KPNs. This can be done by computing a schedule that has to satisfy data dependences within each process, a causality condition for each channel (a message cannot be received before it is sent), and real-time constraints. However, there is a difficulty in writing the channel constraints because one has to count messages in order to establish the send/receive correspondence and, in multi-dimensional loop nests, the counting functions may not be affine. The same situation arises for the OpenStream language (see Section 7.2 .

Recent developments on the theory of polynomials (see Section 7.1) may offer a solution to this problem. One can also define another model, *communicating regular processes* (CRP), in which channels are represented as write-once/read-many arrays. One can then dispense with counting functions and prove that the determinacy property still holds. As an added benefit, a communication system in which the receive operation is not destructive is closer to the expectations of system designers.

The main difficulty with this approach is that ordinary programs are usually not constructed as process networks. One needs automatic or semi-automatic tools for converting sequential programs into process networks. One possibility is to start from array dataflow analysis [15] or variants. Another approach attempts to construct threads, i.e., pieces of sequential code with the smallest possible interactions. In favorable cases, one may even find outermost parallelism, i.e., threads with no interactions whatsoever. Tiling mechanisms can also be used to define atomic processes that can be pipelined as we proposed initially for FPGA [9].

Whatever the chosen solution (FIFO or addressable memory) for communicating between two accelerators or between the host processor and an accelerator, the problems of optimizing communication between processes and of optimizing buffers have to be addressed. Many local memory optimization problems have already been solved theoretically. Some examples are loop fusion and loop alignment for array contraction, techniques for data allocation in scratch-pad memory, or techniques for folding multi-dimensional arrays [11]. Nevertheless, the problem is still largely open. Some questions are: how to schedule a loop sequence (or even a process network) for minimal scratch-pad memory size? How is the problem modified when one introduces unlimited and/or bounded parallelism (same questions for analyzing explicitly-parallel programs)? How does one take into account latency or throughput constraints, bandwidth constraints for input and output channels, memory hierarchies? All loop transformations are useful in this context, in particular loop tiling, and may be applied either as source-to-source transformations (when used in front of HLS or C-level compilers) or to generate directly VHDL or lower-level C-dialects such as OpenCL. One should keep in mind that theory will not be sufficient to solve these problems. Experiments are required to check the relevance of the various models (computation model, memory model, power consumption model) and to select the most important factors according to the architecture. Besides, optimizations do interact: for instance, reducing memory size and increasing parallelism are often antagonistic. Experiments will be needed to find a global compromise between local optimizations. In particular, the design of cost models remain a fundamental challenge.

Finally, there remains the problem of code generation for accelerators. It is a well-known fact that methods for program optimization and parallelization do not generate a new program, but just deliver blueprints for program generation, in the form, e.g., of schedules, placement functions, or new array subscripting functions. A separate code generation phase must be crafted with care, as a too naive implementation may destroy the benefits of high-level optimization. There are two possibilities here as suggested before; one may target another high-level synthesis or compilation tool, or one may target directly VHDL or low-level code. Each approach has its advantages and drawbacks. However, both situations require that the input program respects some strong constraints on the code shape, array accesses, memory accesses, communication protocols, etc. Furthermore, to get the compilers do what the user wants requires a lot of program tuning, i.e., of program rewriting or of program annotations. What can be automated in this rewriting process? Semi-automated?

In other words, we still need to address scheduling, memory, communication, and code generation issues, in the light of the developments of new languages and architectures, pushing the limits of such an automation of program analysis, program optimizations, and code generation.

3.2.2. Beyond Static Control Programs

With the advent of parallelism in supercomputers, the bulk of research in code transformation resulted in (semi-)automatic parallelization, with many techniques (analysis, scheduling, code generation, etc.) based on the description and manipulation of nested loops with polyhedra. Compsys has always taken an active part in the development of these so-called “polyhedral techniques”. Historically, these analysis were (wrongly) understood to be limited to static control programs.

Actually, the polyhedral model is neither a programming language nor an execution model, rather an intermediate representation. As such, it can be generated from imperative sequential languages like C or

Fortran, streaming languages like CRP, or equational languages like Alpha. While the structure of the model is the same in all three cases, it may enjoy different properties, e.g., a schedule always exists in the first case, not in the two others. The import of the polyhedral model is that many questions relative to the analysis of a program and the applicability of transformations can be answered precisely and efficiently by applying well-known mathematical results to the model.

For irregular programs, the basic idea is to construct a polyhedral over-approximation, i.e., a program which has more operations, a larger memory footprint, and more dependences than the original. One can then parallelize the approximated program using polyhedral tools, and then return to the original, either by introducing guards, or by insuring that approximations are harmless. This technique is the standard way of dealing with approximated dependences. We already started to study the impact of approximations in our kernel offloading technique, for optimizing remote communications [10]. It is clear however that this extension method based on over-approximation will apply only to mildly non-polyhedral programs. The restriction to arrays as the only data structure is still present. Its advantage is that it will be able to subsume in a coherent framework many disparate tricks: the extraction of SCoPs, induction variable detection, the omission of non-affine subscripts, or the conversion of control dependences into data dependences. The link with the techniques developed in the PIPS compiler (based on array region analysis) is strong and will have to be explored.

Such over-approximations can be found by mean of abstract interpretation, a general framework to develop static analysis on real-life programs. However, they were designed mainly for verification purposes, thus precision was the main issue before scalability. Although many efforts were made in designing specialized analyses (pointers, data structures, arrays), these approaches still suffer from a lack of experimental evidence concerning their applicability for code optimization. Following our experience and work on termination analysis (that connects the work on back-end CFG-like and front-end polyhedral-like optimizations), and our work on range analysis of numerical variables and on the memory footprint on real-world C programs [18], one of our objectives for the future was to bridge the gap between abstract interpretation and compilation, by designing cheaper analyses that scale well, mainly based on compact representations derived from variants of static single assignment (SSA), with a special focus on complex control, and complex data structures (pointers, lists) that still suffer from complexity issues in the area of optimization.

Another possibility is to rely on application specific knowledge to guide compiler decisions, as it is impossible for a compiler alone to fully exploit such pieces of information. A possible approach to better utilize such knowledge is to put the programmers “in the loop”. Expert parallel programmers often have a good idea about coarse-grain parallelism and locality that they want to use for an application. On the other hand, fine-grain parallelism (e.g., ILP, SIMD) is tedious and specific to each underlying architecture, and is best left to the compiler. Furthermore, approximations will have opportunities to be refined using programmer knowledge. The key challenge is to create a programming environment where compiler techniques and programmer knowledge can be combined effectively. One of the difficulties is to design a common language between the compiler and the programmer. The first step towards this objective is to establish inter-disciplinary collaborations with users, and take the time to analyze and optimize their applications together.M

3.3. Mathematical Tools

All compilers have to deal with *sets* and relations. In classical compilers, these sets are finite: the set of statements of a program, the set of its variables, its abstract syntax tree (AST), its control-flow graph (CFG), and many others. It is only in the first phase of compilation, parsing, that one has to deal with infinite objects, regular and context-free languages, and those are represented by finite grammars, and are processed by a symbolic algorithm, `yacc` or one of its clones.

When tackling parallel programs and parallel compilation, it was soon realized that this position was no longer tenable. Since it makes no sense to ask whether a statement can be executed in parallel with itself, one has to consider sets of operations, which may be so large as to forbid an extensive representation, or even be infinite. The same is true for dependence sets, for memory cells, for communication sets, and for many other objects a parallel compiler has to consider. The representation is to be *symbolic*, and all necessary algorithms have to be promoted to symbolic versions.

Such symbolic representations have to be efficient – the formula representing a set has to be much smaller than the set itself – and effective – the operations one needs, union, intersection, emptiness tests and many others – have to be feasible and fast. As an aside, note that progress in algorithm design has blurred the distinction between polynomially-solvable and NP-complete problems, and between decidable and undecidable questions. For instance SAT, SMT, and ILP software tools solve efficiently many NP-complete problems, and the Z3 tool is able to "solve" many instances of the undecidable Hilbert's 10th problem.

Since the times of Pip and of the Polylib, Compsys has been active in the implementation of basic mathematical tools for program analysis and synthesis. Pip is still developed by Paul Feautrier and Cédric Bastoul, while the Polylib is now taken care of by the Inria Camus project, which introduced Ehrhart polynomials. These tools are still in use world-wide and they also have been reimplemented many times with (sometimes slight) improvements, e.g., as part of the Parma Polylib, of Sven Verdoolaege's Isl and Barvinok libraries, or of the Jollylib of Reservoir Labs. Other groups also made a lot of efforts towards the democratization of the use of polyhedral techniques, in particular the Alchemy Inria project, with Cloog and the development of Graphite in GCC, and Sadayappan's group in the USA, with the development of U. Bondhugula's Pluto prototype compiler. The same effort is made through the PPCG prototype compiler (for GPU) and Pencil (directives-based language on top of PPCG).

After 2009, Compsys continued to focus on the introduction of concepts and techniques to extend the polytope model, with a shift toward tools that may prepare the future. For instance, PoCo and C2fsm are able to parse general programs, not just SCoPs (static control programs), while the efficient handling of Boolean affine formulas [13] is a prerequisite for the construction of non-convex approximations. Euclidean lattices provide an efficient abstraction for the representation of spatial phenomena, and the construction of *critical lattices* as embedded in the tool Cl@k is a first step towards memory optimization in stream languages and may be useful in other situations. Our work on Chuba introduced a new element-wise array reuse analysis and the possibility of handling approximations. Our work on the analysis of while loops is both an extension of the polytope model itself (i.e., beyond SCoPs) and of its applications, here links with program termination and worst-case execution time (WCET) tools.

A recent example of this extension idea is the proposal by Paul Feautrier to use polynomials for program analysis and optimization [14]. The associated tools are based on Handelman and Schweighofer theorems, the polynomial analogue of Farkas lemma. While this is definitely work in progress, with many unsolved questions, it has the potential of greatly enlarging the set of tractable programs.

As a last remark, observe that a common motif of these developments is the transformation of finite algorithms into symbolic algorithms, able to solve very large or even infinite instances. For instance, PIP is a symbolic extension of the Simplex; our work on memory allocation is a symbolic extension of the familiar register allocation problem; loop scheduling extends DAG scheduling. Many other algorithms await their symbolic transformation: a case in point is resource-constrained scheduling.

CONVECS Project-Team

3. Research Program

3.1. New Formal Languages and their Concurrent Implementations

We aim at proposing and implementing new formal languages for the specification, implementation, and verification of concurrent systems. In order to provide a complete, coherent methodological framework, two research directions must be addressed:

- *Model-based specifications*: these are operational (i.e., constructive) descriptions of systems, usually expressed in terms of processes that execute concurrently, synchronize together and communicate. Process calculi are typical examples of model-based specification languages. The approach we promote is based on LOTOS NT (LNT for short), a formal specification language that incorporates most constructs stemming from classical programming languages, which eases its acceptance by students and industry engineers. LNT [29] is derived from the ISO standard E-LOTOS (2001), of which it represents the first successful implementation, based on a source-level translation from LNT to the former ISO standard LOTOS (1989). We are working both on the semantic foundations of LNT (enhancing the language with module interfaces and timed/probabilistic/stochastic features, compiling the m among n synchronization, etc.) and on the generation of efficient parallel and distributed code. Once equipped with these features, LNT will enable formally verified asynchronous concurrent designs to be implemented automatically.
- *Property-based specifications*: these are declarative (i.e., non-constructive) descriptions of systems, which express *what* a system should do rather than *how* the system should do it. Temporal logics and μ-calculi are typical examples of property-based specification languages. The natural models underlying value-passing specification languages, such as LNT, are Labeled Transition Systems (LTSs or simply *graphs*) in which the transitions between states are labeled by actions containing data values exchanged during handshake communications. In order to reason accurately about these LTSs, temporal logics involving data values are necessary. The approach we promote is based on MCL (*Model Checking Language*) [51], which extends the modal μ-calculus with data-handling primitives, fairness operators encoding generalized Büchi automata, and a functional-like language for describing complex transition sequences. We are working both on the semantic foundations of MCL (extending the language with new temporal and hybrid operators, translating these operators into lower-level formalisms, enhancing the type system, etc.) and also on improving the MCL on-the-fly model checking technology (devising new algorithms, enhancing ergonomy by detecting and reporting vacuity, etc.).

We address these two directions simultaneously, yet in a coherent manner, with a particular focus on applicable concurrent code generation and computer-aided verification.

3.2. Parallel and Distributed Verification

Exploiting large-scale high-performance computers is a promising way to augment the capabilities of formal verification. The underlying problems are far from trivial, making the correct design, implementation, fine-tuning, and benchmarking of parallel and distributed verification algorithms long-term and difficult activities. Sequential verification algorithms cannot be reused as such for this task: they are inherently complex, and their existing implementations reflect several years of optimizations and enhancements. To obtain good speedup and scalability, it is necessary to invent new parallel and distributed algorithms rather than to attempt a parallelization of existing sequential ones. We seek to achieve this objective by working along two directions:

- *Rigorous design:* Because of their high complexity, concurrent verification algorithms should themselves be subject to formal modeling and verification, as confirmed by recent trends in the certification of safety-critical applications. To facilitate the development of new parallel and distributed verification algorithms, we promote a rigorous approach based on formal methods and verification. Such algorithms will be first specified formally in LNT, then validated using existing model checking algorithms of the CADP toolbox. Second, parallel or distributed implementations of these algorithms will be generated automatically from the LNT specifications, enabling them to be experimented on large computing infrastructures, such as clusters and grids. As a side-effect, this "bootstrapping" approach would produce new verification tools that can later be used to self-verify their own design.
- *Performance optimization:* In devising parallel and distributed verification algorithms, particular care must be taken to optimize performance. These algorithms will face concurrency issues at several levels: grids of heterogeneous clusters (architecture-independence of data, dynamic load balancing), clusters of homogeneous machines connected by a network (message-passing communication, detection of stable states), and multi-core machines (shared-memory communication, thread synchronization). We will seek to exploit the results achieved in the parallel and distributed computing field to improve performance when using thousands of machines by reducing the number of connections and the messages exchanged between the cooperating processes carrying out the verification task. Another important issue is the generalization of existing LTS representations (explicit, implicit, distributed) in order to make them fully interoperable, such that compilers and verification tools can handle these models transparently.

3.3. Timed, Probabilistic, and Stochastic Extensions

Concurrent systems can be analyzed from a *qualitative* point of view, to check whether certain properties of interest (e.g., safety, liveness, fairness, etc.) are satisfied. This is the role of functional verification, which produces Boolean (yes/no) verdicts. However, it is often useful to analyze such systems from a *quantitative* point of view, to answer non-functional questions regarding performance over the long run, response time, throughput, latency, failure probability, etc. Such questions, which call for numerical (rather than binary) answers, are essential when studying the performance and dependability (e.g., availability, reliability, etc.) of complex systems.

Traditionally, qualitative and quantitative analyzes are performed separately, using different modeling languages and different software tools, often by distinct persons. Unifying these separate processes to form a seamless design flow with common modeling languages and analysis tools is therefore desirable, for both scientific and economic reasons. Technically, the existing modeling languages for concurrent systems need to be enriched with new features for describing quantitative aspects, such as probabilities, weights, and time. Such extensions have been well-studied and, for each of these directions, there exist various kinds of automata, e.g., discrete-time Markov chains for probabilities, weighted automata for weights, timed automata for hard real-time, continuous-time Markov chains for soft real-time with exponential distributions, etc. Nowadays, the next scientific challenge is to combine these individual extensions altogether to provide even more expressive models suitable for advanced applications.

Many such combinations have been proposed in the literature, and there is a large amount of models adding probabilities, weights, and/or time. However, an unfortunate consequence of this diversity is the confuse landscape of software tools supporting such models. Dozens of tools have been developed to implement theoretical ideas about probabilities, weights, and time in concurrent systems. Unfortunately, these tools do not interoperate smoothly, due both to incompatibilities in the underlying semantic models and to the lack of common exchange formats.

To address these issues, CONVECS follows two research directions:

- *Unifying the semantic models.* Firstly, we will perform a systematic survey of the existing semantic models in order to distinguish between their essential and non-essential characteristics, the goal being to propose a unified semantic model that is compatible with process calculi techniques for specifying and verifying concurrent systems. There are already proposals for unification either theoretical (e.g., Markov automata) or practical (e.g., PRISM and MODEST modeling languages), but these languages focus on quantitative aspects and do not provide high-level control structures and data handling features (as LNT does, for instance). Work is therefore needed to unify process calculi and quantitative models, still retaining the benefits of both worlds.

- *Increasing the interoperability of analysis tools*. Secondly, we will seek to enhance the interoperability of existing tools for timed, probabilistic, and stochastic systems. Based on scientific exchanges with developers of advanced tools for quantitative analysis, we plan to evolve the CADP toolbox as follows: extending its perimeter of functional verification with quantitative aspects; enabling deeper connections with external analysis components for probabilistic, stochastic, and timed models; and introducing architectural principles for the design and integration of future tools, our long-term goal being the construction of a European collaborative platform encompassing both functional and non-functional analyzes.

3.4. Component-Based Architectures for On-the-Fly Verification

On-the-fly verification fights against state explosion by enabling an incremental, demand-driven exploration of LTSs, thus avoiding their entire construction prior to verification. In this approach, LTS models are handled implicitly by means of their *post* function, which computes the transitions going out of given states and thus serves as a basis for any forward exploration algorithm. On-the-fly verification tools are complex software artifacts, which must be designed as modularly as possible to enhance their robustness, reduce their development effort, and facilitate their evolution. To achieve such a modular framework, we undertake research in several directions:

- *New interfaces for on-the-fly LTS manipulation*. The current application programming interface (API) for on-the-fly graph manipulation, named OPEN/CAESAR [35], provides an “opaque” representation of states and actions (transitions labels): states are represented as memory areas of fixed size and actions are character strings. Although appropriate to the pure process algebraic setting, this representation must be generalized to provide additional information supporting an efficient construction of advanced verification features, such as: handling of the types, functions, data values, and parallel structure of the source program under verification, independence of transitions in the LTS, quantitative (timed/probabilistic/stochastic) information, etc.
- *Compositional framework for on-the-fly LTS analysis*. On-the-fly model checkers and equivalence checkers usually perform several operations on graph models (LTSs, Boolean graphs, etc.), such as exploration, parallel composition, partial order reduction, encoding of model checking and equivalence checking in terms of Boolean equation systems, resolution and diagnostic generation for Boolean equation systems, etc. To facilitate the design, implementation, and usage of these functionalities, it is necessary to encapsulate them in software components that could be freely combined and replaced. Such components would act as graph transformers, that would execute (on a sequential machine) in a way similar to coroutines and to the composition of lazy functions in functional programming languages. Besides its obvious benefits in modularity, such a component-based architecture will also make it possible to take advantage of multi-core processors.
- *New generic components for on-the-fly verification*. The quest for new on-the-fly components for LTS analysis must be pursued, with the goal of obtaining a rich catalog of interoperable components serving as building blocks for new analysis features. A long-term goal of this approach is to provide an increasingly large catalog of interoperable components covering all verification and analysis functionalities that appear to be useful in practice. It is worth noticing that some components can be very complex pieces of software (e.g., the encapsulation of an on-the-fly model checker for a rich temporal logic). Ideally, it should be possible to build a novel verification or analysis tool by assembling on-the-fly graph manipulation components taken from the catalog. This would provide a flexible means of building new verification and analysis tools by reusing generic, interoperable model manipulation components.

3.5. Real-Life Applications and Case Studies

We believe that theoretical studies and tool developments must be confronted with significant case studies to assess their applicability and to identify new research directions. Therefore, we seek to apply our languages, models, and tools for specifying and verifying formally real-life applications, often in the context of industrial collaborations.

CORSE Project-Team

3. Research Program

3.1. Scientific Foundations

One of the characteristics of CORSE is to base our researches on diverse advanced mathematical tools. Compiler optimization requires the usage of the several tools around discrete mathematics: combinatorial optimization, algorithmic, and graph theory. The aim of CORSE is to tackle optimization not only for regular but also for irregular applications. We believe that new challenges in compiler technology design and in particular for split compilation should also take advantage of graph labeling techniques. In addition to runtime and compiler techniques for program instrumentation, hybrid analysis and compilation advances will be mainly based on polynomial and linear algebra.

The other specificity of CORSE is to address technical challenges related to compiler technology, runtime systems, and hardware characteristics. This implies mastering the details of each. This is especially important as any optimization is based on a reasonably accurate model. Compiler expertise will be used in modeling applications (e.g. through automatic analysis of memory and computational complexity); Runtime expertise will be used in modeling the concurrent activities and overhead due to contention (including memory management); Hardware expertise will be extensively used in modeling physical resources and hardware mechanisms (including synchronization, pipelines, etc.).

The core foundation of the team is related to the combination of static and dynamic techniques, of compilation, and runtime systems. We believe this to be essential in addressing high-performance and low energy challenges in the context of new important changes shown by current application, software, and architecture trends.

Our project is structured along two main directions. The first direction belongs to the area of runtime systems with the objective of developing strong relations with compilers. The second direction belongs to the area of compiler analysis and optimization with the objective of combining dynamic analysis and optimization with static techniques. The aim of CORSE is to ground those two research activities on the development of the end-to-end optimization of some specific domain applications.

DATASHAPE Team

3. Research Program

3.1. Algorithmic aspects of topological and geometric data analysis

TDA requires to construct and manipulate appropriate representations of complex and high dimensional shapes. A major difficulty comes from the fact that the complexity of data structures and algorithms used to approximate shapes rapidly grows as the dimensionality increases, which makes them intractable in high dimensions. We focus our research on simplicial complexes which offer a convenient representation of general shapes and generalize graphs and triangulations. Our work includes the study of simplicial complexes with good approximation properties and the design of compact data structures to represent them.

In low dimensions, effective shape reconstruction techniques exist that can provide precise geometric approximations very efficiently and under reasonable sampling conditions. Extending those techniques to higher dimensions as is required in the context of TDA is problematic since almost all methods in low dimensions rely on the computation of a subdivision of the ambient space. A direct extension of those methods would immediately lead to algorithms whose complexities depend exponentially on the ambient dimension, which is prohibitive in most applications. A first direction to by-pass the curse of dimensionality is to develop algorithms whose complexities depend on the intrinsic dimension of the data (which most of the time is small although unknown) rather than on the dimension of the ambient space. Another direction is to resort to cruder approximations that only captures the homotopy type or the homology of the sampled shape. The recent theory of persistent homology provides a powerful and robust tool to study the homology of sampled spaces in a stable way.

3.2. Statistical aspects of topological and geometric data analysis

The wide variety of larger and larger available data - often corrupted by noise and outliers - requires to consider the statistical properties of their topological and geometric features and to propose new relevant statistical models for their study.

There exist various statistical and machine learning methods intending to uncover the geometric structure of data. Beyond manifold learning and dimensionality reduction approaches that generally do not allow to assert the relevance of the inferred topological and geometric features and are not well-suited for the analysis of complex topological structures, set estimation methods intend to estimate, from random samples, a set around which the data is concentrated. In these methods, that include support and manifold estimation, principal curves/manifolds and their various generalizations to name a few, the estimation problems are usually considered under losses, such as Hausdorff distance or symmetric difference, that are not sensitive to the topology of the estimated sets, preventing these tools to directly infer topological or geometric information.

Regarding purely topological features, the statistical estimation of homology or homotopy type of compact subsets of Euclidean spaces, has only been considered recently, most of the time under the quite restrictive assumption that the data are randomly sampled from smooth manifolds.

In a more general setting, with the emergence of new geometric inference tools based on the study of distance functions and algebraic topology tools such as persistent homology, computational topology has recently seen an important development offering a new set of methods to infer relevant topological and geometric features of data sampled in general metric spaces. The use of these tools remains widely heuristic and until recently there were only a few preliminary results establishing connections between geometric inference, persistent homology and statistics. However, this direction has attracted a lot of attention over the last three years. In particular, stability properties and new representations of persistent homology information have led to very promising results to which the DATASHAPE members have significantly contributed. These preliminary results open many perspectives and research directions that need to be explored.

Our goal is to build on our first statistical results in TDA to develop the mathematical foundations of Statistical Topological and Geometric Data Analysis. Combined with the other objectives, our ultimate goal is to provide a well-founded and effective statistical toolbox for the understanding of topology and geometry of data.

3.3. Topological approach for multimodal data processing

Due to their geometric nature, multimodal data (images, video, 3D shapes, etc.) are of particular interest for the techniques we develop. Our goal is to establish a rigorous framework in which data having different representations can all be processed, mapped and exploited jointly. This requires adapting our tools and sometimes developing entirely new or specialized approaches.

The choice of multimedia data is motivated primarily by the fact that the amount of such data is steadily growing (with e.g. video streaming accounting for nearly two thirds of peak North-American Internet traffic, and almost half a billion images being posted on social networks each day), while at the same time it poses significant challenges in designing informative notions of (dis)-similarity as standard metrics (e.g. Euclidean distances between points) are not relevant.

3.4. Experimental research and software development

We develop a high quality open source software platform called GUDHI which is becoming a reference in geometric and topological data analysis in high dimensions. The goal is not to provide code tailored to the numerous potential applications but rather to provide the central data structures and algorithms that underly applications in geometric and topological data analysis.

The development of the GUDHI platform also serves to benchmark and optimize new algorithmic solutions resulting from our theoretical work. Such development necessitates a whole line of research on software architecture and interface design, heuristics and fine-tuning optimization, robustness and arithmetic issues, and visualization. We aim at providing a full programming environment following the same recipes that made up the success story of the CGAL library, the reference library in computational geometry.

Some of the algorithms implemented on the platform will also be interfaced to other software platform, such as the R software [0] for statistical computing, and languages such as Python in order to make them usable in combination with other data analysis and machine learning tools. A first attempt in this direction has been done with the creation of an R package called TDA in collaboration with the group of Larry Wasserman at Carnegie Mellon University (Inria Associated team CATS) that already includes some functionalities of the GUDHI library and implements some joint results between our team and the CMU team. A similar interface with the Python language is also considered a priority. To go even further towards helping users, we will provide utilities that perform the most common tasks without requiring any programming at all.

[0] https://www.r-project.org/

DEDUCTEAM Team

3. Research Program

3.1. From proof-checking to Interoperability

A new turn with Deduction modulo was taken when the idea of reasoning modulo an arbitrary equivalence relation was applied to typed λ-calculi with dependent types, that permits to express proofs as algorithms, using the Brouwer-Heyting-Kolmogorov interpretation and the Curry-de Bruijn-Howard correspondence [27]. It was shown in 2007, that extending the simplest λ-calculus with dependent types, the $\lambda\Pi$-calculus, with an equivalence relation (more precisely a coingruence), led to a calculus we called the $\lambda\Pi$-calculus modulo, that permitted to simulate many other λ-calculi, such as the Calculus of Constructions, designed to express proofs in specific theories.

This led to the development of a general proof-checker based on the $\lambda\Pi$-calculus modulo [3], that could be used to verify proofs coming from different proof systems, such as Coq [26], HOL [33], etc. To emphasize this versatility of our proof-system, we called it Dedukti —“to deduce” in Esperanto. This system is currently developed together with companion systems, Coqine, Krajono, Holide, Focalide, and Zenonide, that permits to translate proofs from Coq, HOL, Focalize, and Zenon, to Dedukti. Other tools, such as Zenon Modulo, directly output proofs that can be checked by Dedukti. Dedukti proofs can also be exported to other systems, in particular to the MMT format [37].

A thesis, which is at the root of our research effort, and which was already formulated in [32] is that proof-checkers should be theory independent. This is for instance expressed in the title of our invited talk at Icalp 2012: *A theory independent Curry-De Bruijn-Howard correspondence*. Such a theory independent proof-checker is called a *Logical Framework*.

Using a single prover to check proofs coming from different provers naturally led to investigate how these proofs could interact one with another. This issue is of prime importance because developments in proof systems are getting bigger and, unlike other communities in computer science, the proof-checking community has given little effort in the direction of standardization and interoperability. On a longer term we believe that, for each proof, we should be able to identify the systems in which it can be expressed.

3.2. Automated theorem proving

Deduction modulo has originally been proposed to solve a problem in automated theorem proving and some of the early work in this area focused on the design of an automated theorem proving method called *Resolution modulo*, but this method was so complex that it was never implemented. This method was simplified in 2010 [5] and it could then be implemented. This implementation that builds on the iProver effort [36] is called iProver modulo.

iProver modulo gave surprisingly good results [4], so that we use it now to search for proofs in many areas: in the theory of classes—also known as B set theory—, on finite structures, etc. Similar ideas have also been implemented for the tableau method with in particular several extensions of the Zenon automated theorem prover. More precisely, two extensions have been realized: the first one is called SuperZenon [35] [30] and is an extension to superdeduction (which is a variant of Deduction modulo), and the second one is called ZenonModulo [28], [29] and is an extension to Deduction modulo. Both extensions have been extensively tested over first-order problems (of the TPTP library), and also provide good results in terms of number of proved problems. In particular, these tools provide good performances in set theory, so that SuperZenon has been successfully applied to verify B proof rules of Atelier B (work in collaboration with Siemens). Similarly, we plan to apply ZenonModulo in the framework of the BWare project to verify B proof obligations coming from the modeling of industrial applications.

More generally, we believe that proof-checking and automated theorem proving have a lot to learn from each other, because a proof is both a static linguistic object justifying the truth of a proposition and a dynamic process of proving this proposition.

3.3. Models of computation

The idea of Deduction modulo is that computation plays a major role in the foundations of mathematics. This led us to investigate the role played by computation in other sciences, in particular in physics. Some of this work can be seen as a continuation of Gandy's [31] on the fact that the physical Church-Turing thesis is a consequence of three principles of physics, two well-known: the homogeneity of space and time, and the existence of a bound on the velocity of information, and one more speculative: the existence of a bound on the density of information.

This led us to develop physically oriented models of computations.

DICE Team

3. Research Program

3.1. Introduction

Our goal is to address technological issues as well as investigate their impact on society. We believe that addressing both directions simultaneously is essential. More precisely, we focus on the following two objectives:

- Technologies for global intermediation platforms, at reach for unbounded number of users;
- Trans-disciplinary investigations on the global impact of the new intermediation means.

We focus on intermediation platforms, for their increasingly fundamental role in our societies. Intermediation platforms are online systems which offer services to their users, which are well-tuned with their expectation, thanks to the knowledge the platform has accumulated on usage. Search engines and social networks are fundamental examples of intermediation platforms. More generally, intermediation platforms intermediate between producers of services and consumers of services in two-sided markets, with generally one side subsidizing the other. Intermediation will generalise beyond people to things, such as producers or consumers of energy for instance. The capacity to intermediate "in the cloud" with no presence in the physical world in which the market is deployed, by working purely on data with algorithms and in particular learning techniques, is at the heart of the revolution which reshapes our societies.

Platforms ensure a gatekeeping function, always in direct contact with their users, providing them with the most relevant information or contact. They also generate an ecosystem. To do so, platforms allow existing industries as well as new applications proposed by developers to build new services on top of their API. Their impact goes far beyond the Web, while they disrupt step by step all sectors of the economy, transportation, press, education, to name a few.

So far as computer science is concerned, we focus on the technologies used for intermediation, which are at the basis of the largest existing online systems. For the transdisciplinary questions, we focus mostly on the new equilibria that is resulting from the evolution of power balances due mostly to intermediation platforms.

3.2. Intermediation technologies

DICE focuses on intermediation platforms because of the central role they play in the emerging economy.

Intermediation platforms connect users to one another, or users to services with a very high accuracy. They rely on both technological and social innovations. These innovations were unthinkable only a decade ago, when platforms such as Facebook started. They allow communication and interaction between billions of users, gathered in the same digital space, both producers and consumers of data and services. State-of-the-art intermediation platforms include Facebook, Google, Twitter, GitHub, as well as Wikipedia, StackOverflow or Quora. These systems share a common design and their market penetration follows the same pattern. They are built around an initial minimal viable product based on a somehow naive low-tech implementation, which evolves after a few years of improvement to Web giants. Their domination now contributes to standardize the web industry, that means in particular:

- Gatekeeping, a direct relation with users together with services satisfying users' needs;
- Continuous data flows mapped to users' profiles;
- Search engines associating, in a relevant manner, producers, consumers and services.

These common characteristics lead to new software architectural standards, which are shared by all these systems, and used in the peripheral services developed in the ecosystem on top of their API:

- Authentication systems: openId, OAuth, ...
- Object graphs: opengraph, follower/followee scheme, ...
- DataFlow engines: Twitter storm, Google millwheel, ...
- Databases: noSql, keyValues stores, ...
- Application development: javascript, dart, MEAN (Mongo, Express, Angular, Node),...

These architectural components impact the whole digital world. DICE targets systems that use standard architecture services but preserve some aspects we consider as disruptive ones: *data concentration, data symmetry* and *computational subsidiarity*. Our current research activity includes the following directions:

- Peer-to-peer design for preserving users' primary data;
- Third parties based organic systems providing subsidiary data computation hosted at peer sites;
- In-Browser applications that impact mobile device and demonstrate instantaneous usability;
- Flow-based computing enabling a stream based exchange of information between peers at runtime.

3.3. Economy of intermediation

The recent neologism *uberization* coined after the name of *Uber*, a young intermediation platform, may summarize the effects of the digital revolution. This revolution is impacting all sectors of our societies such as organizations, education, energy, transportation and health, to name a few. This revolution results in a serie of what Schumpeter calls *creative destruction*. As traditional sectors disappear, new ones are created. Our societies, which did not anticipate the depth of the changes, have to struggle to adapt to the pace of the development of the industry. Legal reforms in various important sectors including taxation are at stake. Some countries, more reactive than others, are clearly leading the changes, exploiting the benefits for businesses and the capacity to generate information and value, while others are trying to catch up with the global trends.

Data form the bricks of the information society, and their flows between users and services constitute the blood of the industry. We focus in DICE on the strategic role of data in this revolution, and in particular on the systems that harvest the data and concentrate it. In particular, we focus on *intermediation platforms*. Doing so, we investigate the issues they raise and the disruptions they entail.

We are especially interested in the global political impact of intermediation platforms. The settlement of the *right to be forgotten* in Europe, for instance, examplifies the new roles platforms are playing: they are both targets of complaints from institutions and mandatory partners in the governance of the world in the digital era. Indeed, they deeply revolutionize the relations between governments and citizens. If privacy is the focus of considerable attention, together with the state surveillance, in Europe in particular, it is only one aspect of the new knowledge made available. Social media produce considerable knowledge not only on individuals, but on populations as well, their economic fate, their political orientation, etc. On the other hand, open data from governments allow citizens to monitor the action of their governments, as well as to contribute to it. The digital revolution, with the capacity to access information in ways unthinkable in the recent past, modifies completely the balance of powers between citizens, states and corporations.

We investigate the digital world, and more precisely the power relations, from an interdisciplinary perspective. We simultaneously quantify power relations by studying data flows and the rise of intermediation platforms and produce an economical, political and ethical analysis of this new state of affairs. Namely, we show that areas such as the US or China dominate the digital world when others, such as Europe, do not succeed in proposing widely used intermediation platforms. This situation generates several conflicts between countries and companies and prevents *weak* countries from promoting their values and policies.

A new trend is emerging in the humanities, around in particular the digital studies, which promote the cooperation between computer scientists and specialists of social sciences. Among them, the Berkman center for Internet and Society in Harvard, the Medialab at MIT, or the Web Science Institute in the UK have gained strong visibility. They address positive as well as negative externalities of IT for societies, that is the new potentials offered as well as their risks. The Center for Information Technology Research in the Interest of Society in Berkeley also addresses fundamental political impacts on democracy, which can be enhanced by open data as well as another philosophy of political power as currently implemented in the State of California for instance. The Open Data Institute in the UK is also a leading center for political issues in Europe. France should catch up on these research trends, at the intersection of different scientific fields.

DREAMPAL Project-Team

3. Research Program

3.1. New Models for New Technologies

Over the past 25 years there have been several hardware-architecture generations dedicated to massively parallel computing. We have contributed to them in the past, and shall continue doing so in the Dreampal project. The three generations, chronologically ordered, are:

- Supercomputers from the 80s and 90s, based on massively parallel architectures that are more or less distributed (from the Cray T3D or Connection Machine CM2 to GRID 5000). Computer scientists have proposed methods and tools for mapping sequential algorithms to those parallel architectures in order to extract maximum power from them. We have contributed in this area in the past.
- Parallelism pervades the chips! A new challenge appears: hardware/software co-design, in order to obtain performance gains by designing algorithms together with the parallel architectures of chips adapted to the algorithms. During the previous decade many studies, including ours in the Inria DaRT team, were dedicated to this type of co-design. DaRT has contributed to the development of the OMG MARTE standard (http://www.omgmarte.org) and to its implementation on several parallel platforms. Gaspard2, our implementation of this concept, was identified as one of the key software tools developed at Inria: http://www.inria.fr/en/centre/lille/research/platforms-and-flagship-software/flagship-software.
- The new challenge of the 2010s is, in our opinion, the integration of dynamic reconfiguration and massive parallelism. New circuits with high-density integration and supporting dynamic hardware reconfiguration have been proposed. In such architectures one can dynamically change the architecture while an algorithm is running on it. The Dynamic Partial Reconfiguration (DPR) feature offered by recent FPGA boards even allows, in theory, to generate optimized hardware at runtime, by adding, removing, and replacing components on a by-need basis. This integration of dynamic reconfiguration and massive parallelism induces a new degree of complexity, which we, as computer scientists, need to understand and deal with order to make possible the design of applications running on such architectures. This is the main challenge that we address in the Dreampal project. We note that we adress these problems as computer scientists; we do, however, collaborate with electronics specialists in order to benefit from their expertise in 3-D FPGAs.

Excerpt from the HiPEAC vision 2011/12

> *“The advent of 3D stacking enables higher levels of integration and reduced costs for off-chip communications. The overall complexity is managed due to the separation in different dies, independently designed.”*

FPGAs (Field Programmable Gate Arrays) are configurable circuits that have emerged as a privileged target platform for intensive signal processing applications. FPGAs take advantage of the latest technological developments in circuits. For example, the Virtex7 from Xilinx offers a 28-nanometer integration, which is only one or two generations behind the latest general-purpose processors. 3D-Stacked Integrated Circuits (3D SICs) consist of two or more conventional 2D circuits stacked on the top of each other and built into the same IC. Recently, 3D SICs have been released by Xilinx for the Virtex 7 FPGA family. 3D integration will vastly increase the integration capabilities of FPGA circuits. The convergence of massive parallelism and dynamic reconfiguration in inevitable: we believe it is one of the main challenges in computing for the current decade.

By incorporating the configuration and/or data/program memory on the top of the FPGA fabric, with fast and numerous connections between memory and elementary logic blocks (∼10000 connections between dies), it will be possible to obtain dynamically reconfigurable computing platforms with a very high reconfiguration rate. Such a rate was not possible before, due to the serial nature of the interface between the configuration memory and the FPGA fabric itself. The FPGA technology also enables massively parallel architectures due to the large number of programmable logic fabrics available on the chip. For instance, Xilinx demonstrated 3600 8-bit picoBlaze softcore processors running simultaneously on the Virtex-7 2000T FPGA. For specific applications, picoBlaze can be replaced by specialized hardware accelerators or other IPs (Intellectual Property) components. This opens the possibility of creating massively parallel IP-based machines.

3.2. Multi-softcore on 3D FPGA

From the 2010 Xilinx white paper on FPGAs:

> *"Unlike a processor, in which architecture of the ALU is fixed and designed in a general-purpose manner to execute various operations, the CLBs (configurable logic blocks) can be programmed with just the operations needed by the application... The FPGA architecture provides the flexibility to create a massive array of application-specific ALUs..The new solution enables high-bandwidth connectivity between multiple die by providing a much greater number of connections... enabling the integration of massive quantities of interconnect logic resources within a single package"*

Softcore processors are processors implemented using hardware synthesis. Proprietary solutions include PicoBlaze, MicroBlaze, Nios, and Nios II; open-source solutions include Leon, OpenRisk, and FC16. The choice is wide and many new solutions emerge, including multi-softcore implementations on FPGAs. An alternative to softcores are hardware accelerators on FPGAs, which are dedicated circuits that are an order of magnitude faster than softcores. Between these two approaches, there are other various approaches that connect IPs to softcores, in which, the processor's machine-code language is extended, and IP invocations become new instructions. We envisage a new class of softcores (we call them reflective softcores [0]), where almost everything is implemented in IPs; only the control flow is assigned to the softcore itself. The partial dynamic reconfiguration of next-generation FPGAs makes such dynamic IP management possible in practice. We believe that efficient reflective softcores on the new 3D-FPGAs should be as small as possible: low-performance generic hardware components (ALU, registers, memory, I/O...) should be replaced by dedicated high-performance IPs.

We are developing a sofcore processor called HoMade (http://www.lifl.fr/~dekeyser/Homade) following these ideas.

In the multi-reflective softcores that we develop, some softcores will be slaves and others will be masters. Massively parallel dynamically reconfigurable architectures of softcores can thus be envisaged. This requires, additionally, a parallel management of the partial dynamic reconfiguration system. This can be done, for example, on a given subset of softcores: a massively parallel reconfiguration will replace the current replication of a given IP with the replication of a new IP. Thanks to the new 3D-FPGAs this task can be performed efficiently and in parallel using the large number of 3D communication links (Through-Silicon-Vias). Our roadmap for HoMade is to evolve towards this multi-reflective softcore model.

3.3. When Hardware Meets Software

HIPEAC vision 2011/12: *"The number of cores and instruction set extensions increases with every new generation, requiring changes in the software to effectively exploit the new features."*

[0] Hereafter, by reflective system, we mean a system that is able to modify its own structure and behaviour while it is running. A reflective softcore thus dynamically adds, removes, and replaces IPs in the application running on it, and is able to dynamically modify its own program memory, thereby dynamically altering the program it is executing.

When the new massively parallel dynamically reconfigurable architectures become reality users will need languages for programming software applications on them. The languages will be themselves dynamic and parallel, in order to reflect and to fully exploit the dynamicity and parallelism of the architectures. Thus, developers will be able to invoke reconfiguration and call parallel instructions in their programs. This expressiveness comes with a cost, however, because new classes of bugs can be induced by the interaction between dynamic reconfiguration and parallelism; for example, deadlocks due to waiting for output from an IP that does not exist any more due to a reconfiguration. The detection and elimination of such bugs before deployment is paramount for cost-effectiveness and safety reasons.

Thus, we shall build an environment for developing software on parallel, dynamically reconfigurable architectures that will include languages and adequate formal analyses and verification tools for them, in addition to more traditional tools (emulators, compilers, etc). To this end we shall be using formal-semantics frameworks associated with easy-to-use formal verification tools in order to formally define our languages of interest and allow users to formally verify their programs. The K semantic framework (http://k-framework.org), developed jointly by Univs. Urbana Champaign, USA, and Iasi, Romania) is one such framework, which is mature enough (it has allowed defining a formal semantics of the largest subset of the C language to date, as well as many other languages from essentially all programming paradigms) and is familiar to us from previous work. In K, one can rapidly prototype a language definition and try several versions of the syntax and semantics of instructions. This is important in our project, where the proposed programming languages (in particular, the HoMade assembly language) will go through several versions before being stabilized. Moreover, once a language is defined in K one gets an interpreter of the language and one gains access to formal verification tools for free. We are also developing new analysis verification tools for K (in collaboration with the K team), which will be adapted and used in the Dreampal project.

GALLIUM Project-Team

3. Research Program

3.1. Programming languages: design, formalization, implementation

Like all languages, programming languages are the media by which thoughts (software designs) are communicated (development), acted upon (program execution), and reasoned upon (validation). The choice of adequate programming languages has a tremendous impact on software quality. By “adequate”, we mean in particular the following four aspects of programming languages:

- **Safety.** The programming language must not expose error-prone low-level operations (explicit memory deallocation, unchecked array access, etc) to programmers. Further, it should provide constructs for describing data structures, inserting assertions, and expressing invariants within programs. The consistency of these declarations and assertions should be verified through compile-time verification (e.g. static type-checking) and run-time checks.
- **Expressiveness.** A programming language should manipulate as directly as possible the concepts and entities of the application domain. In particular, complex, manual encodings of domain notions into programmatic notations should be avoided as much as possible. A typical example of a language feature that increases expressiveness is pattern matching for examination of structured data (as in symbolic programming) and of semi-structured data (as in XML processing). Carried to the extreme, the search for expressiveness leads to domain-specific languages, customized for a specific application area.
- **Modularity and compositionality.** The complexity of large software systems makes it impossible to design and develop them as one, monolithic program. Software decomposition (into semi-independent components) and software composition (of existing or independently-developed components) are therefore crucial. Again, this modular approach can be applied to any programming language, given sufficient fortitude by the programmers, but is much facilitated by adequate linguistic support. In particular, reflecting notions of modularity and software components in the programming language enables compile-time checking of correctness conditions such as type correctness at component boundaries.
- **Formal semantics.** A programming language should fully and formally specify the behaviours of programs using mathematical semantics, as opposed to informal, natural-language specifications. Such a formal semantics is required in order to apply formal methods (program proof, model checking) to programs.

Our research work in language design and implementation centers on the statically-typed functional programming paradigm, which scores high on safety, expressiveness and formal semantics, complemented with full imperative features and objects for additional expressiveness, and modules and classes for compositionality. The OCaml language and system embodies many of our earlier results in this area [49]. Through collaborations, we also gained experience with several domain-specific languages based on a functional core, including distributed programming (JoCaml), XML processing (XDuce, CDuce), reactive functional programming, and hardware modeling.

3.2. Type systems

Type systems [52] are a very effective way to improve programming language reliability. By grouping the data manipulated by the program into classes called types, and ensuring that operations are never applied to types over which they are not defined (e.g. accessing an integer as if it were an array, or calling a string as if it were a function), a tremendous number of programming errors can be detected and avoided, ranging from the trivial (misspelled identifier) to the fairly subtle (violation of data structure invariants). These restrictions are also very effective at thwarting basic attacks on security vulnerabilities such as buffer overflows.

The enforcement of such typing restrictions is called type-checking, and can be performed either dynamically (through run-time type tests) or statically (at compile-time, through static program analysis). We favor static type-checking, as it catches bugs earlier and even in rarely-executed parts of the program, but note that not all type constraints can be checked statically if static type-checking is to remain decidable (i.e. not degenerate into full program proof). Therefore, all typed languages combine static and dynamic type-checking in various proportions.

Static type-checking amounts to an automatic proof of partial correctness of the programs that pass the compiler. The two key words here are *partial*, since only type safety guarantees are established, not full correctness; and *automatic*, since the proof is performed entirely by machine, without manual assistance from the programmer (beyond a few, easy type declarations in the source). Static type-checking can therefore be viewed as the poor man's formal methods: the guarantees it gives are much weaker than full formal verification, but it is much more acceptable to the general population of programmers.

3.2.1. Type systems and language design.

Unlike most other uses of static program analysis, static type-checking rejects programs that it cannot prove safe. Consequently, the type system is an integral part of the language design, as it determines which programs are acceptable and which are not. Modern typed languages go one step further: most of the language design is determined by the *type structure* (type algebra and typing rules) of the language and intended application area. This is apparent, for instance, in the XDuce and CDuce domain-specific languages for XML transformations [46], [43], whose design is driven by the idea of regular expression types that enforce DTDs at compile-time. For this reason, research on type systems – their design, their proof of semantic correctness (type safety), the development and proof of associated type-checking and inference algorithms – plays a large and central role in the field of programming language research, as evidenced by the huge number of type systems papers in conferences such as Principles of Programming Languages.

3.2.2. Polymorphism in type systems.

There exists a fundamental tension in the field of type systems that drives much of the research in this area. On the one hand, the desire to catch as many programming errors as possible leads to type systems that reject more programs, by enforcing fine distinctions between related data structures (say, sorted arrays and general arrays). The downside is that code reuse becomes harder: conceptually identical operations must be implemented several times (say, copying a general array and a sorted array). On the other hand, the desire to support code reuse and to increase expressiveness leads to type systems that accept more programs, by assigning a common type to broadly similar objects (for instance, the `Object` type of all class instances in Java). The downside is a loss of precision in static typing, requiring more dynamic type checks (downcasts in Java) and catching fewer bugs at compile-time.

Polymorphic type systems offer a way out of this dilemma by combining precise, descriptive types (to catch more errors statically) with the ability to abstract over their differences in pieces of reusable, generic code that is concerned only with their commonalities. The paradigmatic example is parametric polymorphism, which is at the heart of all typed functional programming languages. Many forms of polymorphic typing have been studied since then. Taking examples from our group, the work of Rémy, Vouillon and Garrigue on row polymorphism [55], integrated in OCaml, extended the benefits of this approach (reusable code with no loss of typing precision) to object-oriented programming, extensible records and extensible variants. Another example is the work by Pottier on subtype polymorphism, using a constraint-based formulation of the type system [53]. Finally, the notion of "coercion polymorphism" proposed by Cretin and Rémy[3] combines and generalizes both parametric and subtyping polymorphism.

3.2.3. Type inference.

Another crucial issue in type systems research is the issue of type inference: how many type annotations must be provided by the programmer, and how many can be inferred (reconstructed) automatically by the type-checker? Too many annotations make the language more verbose and bother the programmer with unnecessary details. Too few annotations make type-checking undecidable, possibly requiring heuristics, which is unsatisfactory. OCaml requires explicit type information at data type declarations and at component interfaces, but infers all other types.

In order to be predictable, a type inference algorithm must be complete. That is, it must not find *one*, but *all* ways of filling in the missing type annotations to form an explicitly typed program. This task is made easier when all possible solutions to a type inference problem are *instances* of a single, *principal* solution.

Maybe surprisingly, the strong requirements – such as the existence of principal types – that are imposed on type systems by the desire to perform type inference sometimes lead to better designs. An illustration of this is row variables. The development of row variables was prompted by type inference for operations on records. Indeed, previous approaches were based on subtyping and did not easily support type inference. Row variables have proved simpler than structural subtyping and more adequate for type-checking record update, record extension, and objects.

Type inference encourages abstraction and code reuse. A programmer's understanding of his own program is often initially limited to a particular context, where types are more specific than strictly required. Type inference can reveal the additional generality, which allows making the code more abstract and thus more reuseable.

3.3. Compilation

Compilation is the automatic translation of high-level programming languages, understandable by humans, to lower-level languages, often executable directly by hardware. It is an essential step in the efficient execution, and therefore in the adoption, of high-level languages. Compilation is at the interface between programming languages and computer architecture, and because of this position has had considerable influence on the design of both. Compilers have also attracted considerable research interest as the oldest instance of symbolic processing on computers.

Compilation has been the topic of much research work in the last 40 years, focusing mostly on high-performance execution ("optimization") of low-level languages such as Fortran and C. Two major results came out of these efforts: one is a superb body of performance optimization algorithms, techniques and methodologies; the other is the whole field of static program analysis, which now serves not only to increase performance but also to increase reliability, through automatic detection of bugs and establishment of safety properties. The work on compilation carried out in the Gallium group focuses on a less investigated topic: compiler certification.

3.3.1. Formal verification of compiler correctness.

While the algorithmic aspects of compilation (termination and complexity) have been well studied, its semantic correctness – the fact that the compiler preserves the meaning of programs – is generally taken for granted. In other terms, the correctness of compilers is generally established only through testing. This is adequate for compiling low-assurance software, themselves validated only by testing: what is tested is the executable code produced by the compiler, therefore compiler bugs are detected along with application bugs. This is not adequate for high-assurance, critical software which must be validated using formal methods: what is formally verified is the source code of the application; bugs in the compiler used to turn the source into the final executable can invalidate the guarantees so painfully obtained by formal verification of the source.

To establish strong guarantees that the compiler can be trusted not to change the behavior of the program, it is necessary to apply formal methods to the compiler itself. Several approaches in this direction have been investigated, including translation validation, proof-carrying code, and type-preserving compilation. The approach that we currently investigate, called *compiler verification*, applies program proof techniques to the compiler itself, seen as a program in particular, and use a theorem prover (the Coq system) to prove that the generated code is observationally equivalent to the source code. Besides its potential impact on the critical software industry, this line of work is also scientifically fertile: it improves our semantic understanding of compiler intermediate languages, static analyses and code transformations.

3.4. Interface with formal methods

Formal methods collectively refer to the mathematical specification of software or hardware systems and to the verification of these systems against these specifications using computer assistance: model checkers, theorem provers, program analyzers, etc. Despite their costs, formal methods are gaining acceptance in the critical software industry, as they are the only way to reach the required levels of software assurance.

In contrast with several other Inria projects, our research objectives are not fully centered around formal methods. However, our research intersects formal methods in the following two areas, mostly related to program proofs using proof assistants and theorem provers.

3.4.1. Software-proof codesign

The current industrial practice is to write programs first, then formally verify them later, often at huge costs. In contrast, we advocate a codesign approach where the program and its proof of correctness are developed in interaction, and we are interested in developing ways and means to facilitate this approach. One possibility that we currently investigate is to extend functional programming languages such as OCaml with the ability to state logical invariants over data structures and pre- and post-conditions over functions, and interface with automatic or interactive provers to verify that these specifications are satisfied. Another approach that we practice is to start with a proof assistant such as Coq and improve its capabilities for programming directly within Coq.

3.4.2. Mechanized specifications and proofs for programming languages components

We emphasize mathematical specifications and proofs of correctness for key language components such as semantics, type systems, type inference algorithms, compilers and static analyzers. These components are getting so large that machine assistance becomes necessary to conduct these mathematical investigations. We have already mentioned using proof assistants to verify compiler correctness. We are also interested in using them to specify and reason about semantics and type systems. These efforts are part of a more general research topic that is gaining importance: the formal verification of the tools that participate in the construction and certification of high-assurance software.

GRACE Project-Team

3. Research Program

3.1. Algorithmic Number Theory

Algorithmic Number Theory is concerned with replacing special cases with general algorithms to solve problems in number theory. In the Grace project, it appears in three main threads:

- fundamental algorithms for integers and polynomials (including primality and factorization);
- algorithms for finite fields (including discrete logarithms); and
- algorithms for algebraic curves.

Clearly, we use computer algebra in many ways. Research in cryptology has motivated a renewed interest in Algorithmic Number Theory in recent decades—but the fundamental problems still exist *per se*. Indeed, while algorithmic number theory application in cryptanalysis is epitomized by applying factorization to breaking RSA public key, many other problems, are relevant to various area of computer science. Roughly speaking, the problems of the cryptological world are of bounded size, whereas Algorithmic Number Theory is also concerned with asymptotic results.

3.2. Arithmetic Geometry: Curves and their Jacobians

Theme: Arithmetic Geometry: Curves and their Jacobians *Arithmetic Geometry* is the meeting point of algebraic geometry and number theory: that is, the study of geometric objects defined over arithmetic number systems (such as the integers and finite fields). The fundamental objects for our applications in both coding theory and cryptology are curves and their Jacobians over finite fields.

An algebraic *plane curve*$\mathcal{X}$ over a field $\mathbf{K}$ is defined by an equation

$$\mathcal{X} : F_{\mathcal{X}}(x, y) = 0 \quad \text{where } F_{\mathcal{X}} \in \mathbf{K}[x, y].$$

(Not every curve is planar—we may have more variables, and more defining equations—but from an algorithmic point of view, we can always reduce to the plane setting.) The *genus*$g_{\mathcal{X}}$ of $\mathcal{X}$ is a non-negative integer classifying the essential geometric complexity of $\mathcal{X}$; it depends on the degree of $F_{\mathcal{X}}$ and on the number of singularities of $\mathcal{X}$. The curve $\mathcal{X}$ is associated in a functorial way with an algebraic group $J_{\mathcal{X}}$, called the *Jacobian* of $\mathcal{X}$. The group $J_{\mathcal{X}}$ has a geometric structure: its elements correspond to points on a $g_{\mathcal{X}}$-dimensional projective algebraic group variety. Typically, we do not compute with the equations defining this projective variety: there are too many of them, in too many variables, for this to be convenient. Instead, we use fast algorithms based on the representation in terms of classes of formal sums of points on $\mathcal{X}$.

The simplest curves with nontrivial Jacobians are curves of genus 1, known as *elliptic curves*; they are typically defined by equations of the form $y^2 = x^3 + Ax + B$. Elliptic curves are particularly important given their central role in public-key cryptography over the past two decades. Curves of higher genus are important in both cryptography and coding theory.

3.3. Curve-Based cryptology

Theme: Curve-Based Cryptology

Jacobians of curves are excellent candidates for cryptographic groups when constructing efficient instances of public-key cryptosystems. Diffie–Hellman key exchange is an instructive example.

Suppose Alice and Bob want to establish a secure communication channel. Essentially, this means establishing a common secret *key*, which they will then use for encryption and decryption. Some decades ago, they would have exchanged this key in person, or through some trusted intermediary; in the modern, networked world, this is typically impossible, and in any case completely unscalable. Alice and Bob may be anonymous parties who want to do e-business, for example, in which case they cannot securely meet, and they have no way to be sure of each other's identities. Diffie–Hellman key exchange solves this problem. First, Alice and Bob publicly agree on a cryptographic group G with a generator P (of order N); then Alice secretly chooses an integer a from $[1..N]$, and sends aP to Bob. In the meantime, Bob secretly chooses an integer b from $[1..N]$, and sends bP to Alice. Alice then computes $a(bP)$, while Bob computes $b(aP)$; both have now computed abP, which becomes their shared secret key. The security of this key depends on the difficulty of computing abP given P, aP, and bP; this is the Computational Diffie–Hellman Problem (CDHP). In practice, the CDHP corresponds to the Discrete Logarithm Problem (DLP), which is to determine a given P and aP.

This simple protocol has been in use, with only minor modifications, since the 1970s. The challenge is to create examples of groups G with a relatively compact representation and an efficiently computable group law, and such that the DLP in G is hard (ideally approaching the exponential difficulty of the DLP in an abstract group). The Pohlig–Hellman reduction shows that the DLP in G is essentially only as hard as the DLP in its largest prime-order subgroup. We therefore look for compact and efficient groups of prime order.

The classic example of a group suitable for the Diffie–Hellman protocol is the multiplicative group of a finite field $\mathbf{F}_q$. There are two problems that render its usage somewhat less than ideal. First, it has too much structure: we have a subexponential Index Calculus attack on the DLP in this group, so while it is very hard, the DLP falls a long way short of the exponential difficulty of the DLP in an abstract group. Second, there is only one such group for each q: its subgroup treillis depends only on the factorization of $q - 1$, and requiring $q - 1$ to have a large prime factor eliminates many convenient choices of q.

This is where Jacobians of algebraic curves come into their own. First, elliptic curves and Jacobians of genus 2 curves do not have a subexponential index calculus algorithm: in particular, from the point of view of the DLP, a generic elliptic curve is currently *as strong as* a generic group of the same size. Second, they provide some diversity: we have many degrees of freedom in choosing curves over a fixed $\mathbf{F}_q$, with a consequent diversity of possible cryptographic group orders. Furthermore, an attack which leaves one curve vulnerable may not necessarily apply to other curves. Third, viewing a Jacobian as a geometric object rather than a pure group allows us to take advantage of a number of special features of Jacobians. These features include efficiently computable pairings, geometric transformations for optimised group laws, and the availability of efficiently computable non-integer endomorphisms for accelerated encryption and decryption.

3.4. Algebraic Coding Theory

Theme: Coding theory

Coding Theory studies originated with the idea of using redundancy in messages to protect against noise and errors. The last decade of the 20th century has seen the success of so-called iterative decoding methods, which enable us to get very close to the Shannon capacity. The capacity of a given channel is the best achievable transmission rate for reliable transmission. The consensus in the community is that this capacity is more easily reached with these iterative and probabilistic methods than with algebraic codes (such as Reed–Solomon codes).

However, algebraic coding is useful in settings other than the Shannon context. Indeed, the Shannon setting is a random case setting, and promises only a vanishing error probability. In contrast, the algebraic Hamming approach is a worst case approach: under combinatorial restrictions on the noise, the noise can be adversarial, with strictly zero errors.

These considerations are renewed by the topic of list decoding after the breakthrough of Guruswami and Sudan at the end of the nineties. List decoding relaxes the uniqueness requirement of decoding, allowing a small list of candidates to be returned instead of a single codeword. List decoding can reach a capacity close to the Shannon capacity, with zero failure, with small lists, in the adversarial case. The method of

Guruswami and Sudan enabled list decoding of most of the main algebraic codes: Reed–Solomon codes and Algebraic–Geometry (AG) codes and new related constructions "capacity-achieving list decodable codes". These results open the way to applications again adversarial channels, which correspond to worst case settings in the classical computer science language.

Another avenue of our studies is AG codes over various geometric objects. Although Reed–Solomon codes are the best possible codes for a given alphabet, they are very limited in their length, which cannot exceed the size of the alphabet. AG codes circumvent this limitation, using the theory of algebraic curves over finite fields to construct long codes over a fixed alphabet. The striking result of Tsfasman–Vladut–Zink showed that codes better than random codes can be built this way, for medium to large alphabets. Disregarding the asymptotic aspects and considering only finite length, AG codes can be used either for longer codes with the same alphabet, or for codes with the same length with a smaller alphabet (and thus faster underlying arithmetic).

From a broader point of view, wherever Reed–Solomon codes are used, we can substitute AG codes with some benefits: either beating random constructions, or beating Reed–Solomon codes which are of bounded length for a given alphabet.

Another area of Algebraic Coding Theory with which we are more recently concerned is the one of Locally Decodable Codes. After having been first theoretically introduced, those codes now begin to find practical applications, most notably in cloud-based remote storage systems.

HYCOMES Project-Team

3. Research Program

3.1. Hybrid Systems Modeling

Systems industries today make extensive use of mathematical modeling tools to design computer controlled physical systems. This class of tools addresses the modeling of physical systems with models that are simpler than usual scientific computing problems by using only Ordinary Differential Equations (ODE) and Difference Equations but not Partial Differential Equations (PDE). This family of tools first emerged in the 1980's with SystemBuild by MatrixX (now distributed by National Instruments) followed soon by Simulink by Mathworks, with an impressive subsequent development.

In the early 90's control scientists from the University of Lund (Sweden) realized that the above approach did not support component based modeling of physical systems with reuse [0]. For instance, it was not easy to draw an electrical or hydraulic circuit by assembling component models of the various devices. The development of the Omola language by Hilding Elmqvist was a first attempt to bridge this gap by supporting some form of Differential Algebraic Equations (DAE) in the models. Modelica quickly emerged from this first attempt and became in the 2000's a major international concerted effort with the Modelica Consortium [0]. A wider set of tools, both industrial and academic, now exists in this segment [0]. In the EDA sector, VHDL-AMS was developed as a standard [13].

Despite these tools are now widely used by a number of engineers, they raise a number of technical difficulties. The meaning of some programs, their mathematical semantics, can be tainted with uncertainty. A main source of difficulty lies in the failure to properly handle the discrete and the continuous parts of systems, and their interaction. How the propagation of mode changes and resets should be handled? How to avoid artifacts due to the use of a global ODE solver causing unwanted coupling between seemingly non interacting subsystems? Also, the mixed use of an equational style for the continuous dynamics with an imperative style for the mode changes and resets is a source of difficulty when handling parallel composition. It is therefore not uncommon that tools return complex warnings for programs with many different suggested hints for fixing them. Yet, these "pathological" programs can still be executed, if wanted so, giving surprising results — See for instance the Simulink examples in [21], [1] and [17].

Indeed this area suffers from the same difficulties that led to the development of the theory of synchronous languages as an effort to fix obscure compilation schemes for discrete time equation based languages in the 1980's. Our vision is that hybrid systems modeling tools deserve similar efforts in theory as synchronous languages did for the programming of embedded systems.

3.2. Background on non-standard analysis

Non-Standard analysis plays a central role in our research on hybrid systems modeling [1], [21], [18], [17]. The following text provides a brief summary of this theory and gives some hints on its usefulness in the context of hybrid systems modeling. This presentation is based on our paper [1], a chapter of Simon Bliudze's PhD thesis [27], and a recent presentation of non-standard analysis, not axiomatic in style, due to the mathematician Lindström [50].

[0] http://www.lccc.lth.se/media/LCCC2012/WorkshopSeptember/slides/Astrom.pdf

[0] https://www.modelica.org/

[0] SimScape by Mathworks, Amesim by LMS International, now Siemens PLM, and more.

Non-standard numbers allowed us to reconsider the semantics of hybrid systems and propose a radical alternative to the *super-dense time semantics* developed by Edward Lee and his team as part of the Ptolemy II project, where cascades of successive instants can occur in zero time by using $\mathbb{R}_+ \times \mathbb{N}$ as a time index. In the non-standard semantics, the time index is defined as a set $\mathbb{T} = \{n\partial \mid n \in {}^*\mathbb{N}\}$, where ∂ is an *infinitesimal* and ${}^*\mathbb{N}$ is the set of *non-standard integers*. Remark that 1/ $\mathbb{T}$ is dense in $\mathbb{R}_+$, making it "continuous", and 2/ every $t \in \mathbb{T}$ has a predecessor in $\mathbb{T}$ and a successor in $\mathbb{T}$, making it "discrete". Although it is not effective from a computability point of view, the *non-standard semantics* provides a framework that is familiar to the computer scientist and at the same time efficient as a symbolic abstraction. This makes it an excellent candidate for the development of provably correct compilation schemes and type systems for hybrid systems modeling languages.

Non-standard analysis was proposed by Abraham Robinson in the 1960s to allow the explicit manipulation of "infinitesimals" in analysis [56], [42], [12]. Robinson's approach is axiomatic; he proposes adding three new axioms to the basic Zermelo-Fraenkel (ZFC) framework. There has been much debate in the mathematical community as to whether it is worth considering non-standard analysis instead of staying with the traditional one. We do not enter this debate. The important thing for us is that non-standard analysis allows the use of the non-standard discretization of continuous dynamics "as if" it was operational.

Not surprisingly, such an idea is quite ancient. Iwasaki et al. [46] first proposed using non-standard analysis to discuss the nature of time in hybrid systems. Bliudze and Krob [28], [27] have also used non-standard analysis as a mathematical support for defining a system theory for hybrid systems. They discuss in detail the notion of "system" and investigate computability issues. The formalization they propose closely follows that of Turing machines, with a memory tape and a control mechanism.

The introduction to non-standard analysis in [27] is very pleasant and we take the liberty to borrow it. This presentation was originally due to Lindstrøm, see [50]. Its interest is that it does not require any fancy axiomatic material but only makes use of the axiom of choice — actually a weaker form of it. The proposed construction bears some resemblance to the construction of $\mathbb{R}$ as the set of equivalence classes of Cauchy sequences in $\mathbb{Q}$ modulo the equivalence relation $(u_n) \approx (v_n)$ iff $\lim_{n\to\infty}(u_n - v_n) = 0$.

3.3. Contract-Based Design, Interfaces Theories, and Requirements Engineering

System companies such as automotive and aeronautic companies are facing significant difficulties due to the exponentially raising complexity of their products coupled with increasingly tight demands on functionality, correctness, and time-to-market. The cost of being late to market or of imperfections in the products is staggering as witnessed by the recent recalls and delivery delays that many major car and airplane manufacturers had to bear in the recent years. The specific root causes of these design problems are complex and relate to a number of issues ranging from design processes and relationships with different departments of the same company and with suppliers, to incomplete requirement specification and testing.

We believe the most promising means to address the challenges in systems engineering is to employ structured and formal design methodologies that seamlessly and coherently combine the various viewpoints of the design space (behavior, space, time, energy, reliability, ...), that provide the appropriate abstractions to manage the inherent complexity, and that can provide correct-by-construction implementations. The following technology issues must be addressed when developing new approaches to the design of complex systems:

- The overall design flows for heterogeneous systems and the associated use of models across traditional boundaries are not well developed and understood. Relationships between different teams inside a same company, or between different stake-holders in the supplier chain, are not well supported by solid technical descriptions for the mutual obligations.
- System requirements capture and analysis is in large part a heuristic process, where the informal text and natural language-based techniques in use today are facing significant challenges. Formal requirements engineering is in its infancy: mathematical models, formal analysis techniques and links to system implementation must be developed.

- Dealing with variability, uncertainty, and life-cycle issues, such as extensibility of a product family, are not well-addressed using available systems engineering methodologies and tools.

The challenge is to address the entire process and not to consider only local solutions of methodology, tools, and models that ease part of the design.

Contract-based design has been proposed as a new approach to the system design problem that is rigorous and effective in dealing with the problems and challenges described before, and that, at the same time, does not require a radical change in the way industrial designers carry out their task as it cuts across design flows of different type. Indeed, contracts can be used almost everywhere and at nearly all stages of system design, from early requirements capture, to embedded computing infrastructure and detailed design involving circuits and other hardware. Contracts explicitly handle pairs of properties, respectively representing the assumptions on the environment and the guarantees of the system under these assumptions. Intuitively, a contract is a pair $C = (A, G)$ of assumptions and guarantees characterizing in a formal way 1) under which context the design is assumed to operate, and 2) what its obligations are. Assume/Guarantee reasoning has been known for a long time, and has been used mostly as verification mean for the design of software [54]. However, contract based design with explicit assumptions is a philosophy that should be followed all along the design, with all kinds of models, whenever necessary. Here, specifications are not limited to profiles, types, or taxonomy of data, but also describe the functions, performances of various kinds (time and energy), and reliability. This amounts to enrich a component's interface with, on one hand, formal specifications of the behavior of the environment in which the component may be instantiated and, on the other hand, of the expected behavior of the component itself. The consideration of rich interfaces is still in its infancy. So far, academic researchers have addressed the mathematics and algorithmics of interfaces theories and contract-based reasoning. To make them a technique of choice for system engineers, we must develop:

- Mathematical foundations for interfaces and requirements engineering that enable the design of frameworks and tools;
- A system engineering framework and associated methodologies and tool sets that focus on system requirements modeling, contract specification, and verification at multiple abstraction layers.

A detailed bibliography on contract and interface theories for embedded system design can be found in [2]. In a nutshell, contract and interface theories fall into two main categories:

Assume/guarantee contracts. By explicitly relying on the notions of assumptions and guarantees, A/G-contracts are intuitive, which makes them appealing for the engineer. In A/G-contracts, assumptions and guarantees are just properties regarding the behavior of a component and of its environment. The typical case is when these properties are formal languages or sets of traces, which includes the class of safety properties [47], [36], [53], [15], [37]. Contract theories were initially developed as specification formalisms able to refuse some inputs from the environment [43]. A/G-contracts were advocated by the SPEEDS project [20]. They were further experimented in the framework of the CESAR project [38], with the additional consideration of *weak* and *strong* assumptions. This is still a very active research topic, with several recent contributions dealing with the timed [25] and probabilistic [32], [33] viewpoints in system design, and even mixed-analog circuit design [55].

Automata theoretic interfaces. Interfaces combine assumptions and guarantees in a single, automata theoretic specification. Most interface theories are based on Lynch Input/Output Automata [52], [51]. Interface Automata [59], [58], [60], [34] focus primarily on parallel composition and compatibility: Two interfaces can be composed and are compatible if there is at least one environment where they can work together. The idea is that the resulting composition exposes as an interface the needed information to ensure that incompatible pairs of states cannot be reached. This can be achieved by using the possibility, for an Interface Automaton, to refuse selected inputs from the environment in a given state, which amounts to the implicit assumption that the environment will never produce any of the refused inputs, when the interface is in this state. Modal Interfaces [3] inherit from both Interface Automata and the originally unrelated notion of Modal Transition System [49], [14], [29], [48]. Modal Interfaces are strictly more expressive than Interface Automata by decoupling the I/O orientation of an event and its deontic modalities (mandatory, allowed or forbidden). Informally, a *must* transition is available in every component that realizes the modal interface, while a *may* transition needs not be. Research on interface theories is still very active. For instance, timed [61], [22], [24], [40], [39], [23], probabilistic [32], [41] and energy-aware [35] interface theories have been proposed recently.

Requirements Engineering is one of the major concerns in large systems industries today, particularly so in sectors where certification prevails [57]. DOORS projects collecting requirements are poorly structured and cannot be considered a formal modeling framework today. They are nothing more than an informal documentation enriched with hyperlinks. As examples, medium size sub-systems may have a few thousands requirements and the Rafale fighter aircraft has above 250,000 of them. For the Boeing 787, requirements were not stable while subcontractors performed the development of the fly-by-wire and of the landing gear subsystems.

We see Contract-Based Design and Interfaces Theories as innovative tools in support of Requirements Engineering. The Software Engineering community has extensively covered several aspects of Requirements Engineering, in particular:

- the development and use of large and rich *ontologies*; and
- the use of Model Driven Engineering technology for the structural aspects of requirements and resulting hyperlinks (to tests, documentation, PLM, architecture, and so on).

Behavioral models and properties, however, are not properly encompassed by the above approaches. This is the cause of a remaining gap between this phase of systems design and later phases where formal model based methods involving behavior have become prevalent—see the success of Matlab/Simulink/Scade technologies. We believe that our work on contract based design and interface theories is best suited to bridge this gap.

LFANT Project-Team

3. Research Program

3.1. Number fields, class groups and other invariants

Participants: Bill Allombert, Karim Belabas, Cyril Bouvier, Jean-Paul Cerri, Iuliana Ciocanea-Teodorescu, Henri Cohen, Jean-Marc Couveignes, Andreas Enge, Fredrik Johansson, Pınar Kılıçer.

Modern number theory has been introduced in the second half of the 19th century by Dedekind, Kummer, Kronecker, Weber and others, motivated by Fermat's conjecture: There is no non-trivial solution in integers to the equation $x^n + y^n = z^n$ for $n \geqslant 3$. For recent textbooks, see [5]. Kummer's idea for solving Fermat's problem was to rewrite the equation as $(x+y)(x+\zeta y)(x+\zeta^2 y)\cdots(x+\zeta^{n-1}y) = z^n$ for a primitive n-th root of unity ζ, which seems to imply that each factor on the left hand side is an n-th power, from which a contradiction can be derived.

The solution requires to augment the integers by *algebraic numbers*, that are roots of polynomials in $\mathbb{Z}[X]$. For instance, ζ is a root of $X^n - 1$, $\sqrt[3]{2}$ is a root of $X^3 - 2$ and $\frac{\sqrt{3}}{5}$ is a root of $25X^2 - 3$. A *number field* consists of the rationals to which have been added finitely many algebraic numbers together with their sums, differences, products and quotients. It turns out that actually one generator suffices, and any number field K is isomorphic to $\mathbb{Q}[X]/(f(X))$, where $f(X)$ is the minimal polynomial of the generator. Of special interest are *algebraic integers*, "numbers without denominators", that are roots of a monic polynomial. For instance, ζ and $\sqrt[3]{2}$ are integers, while $\frac{\sqrt{3}}{5}$ is not. The *ring of integers* of K is denoted by $\mathcal{O}_K$; it plays the same role in K as $\mathbb{Z}$ in $\mathbb{Q}$.

Unfortunately, elements in $\mathcal{O}_K$ may factor in different ways, which invalidates Kummer's argumentation. Unique factorisation may be recovered by switching to *ideals*, subsets of $\mathcal{O}_K$ that are closed under addition and under multiplication by elements of $\mathcal{O}_K$. In $\mathbb{Z}$, for instance, any ideal is *principal*, that is, generated by one element, so that ideals and numbers are essentially the same. In particular, the unique factorisation of ideals then implies the unique factorisation of numbers. In general, this is not the case, and the *class group*Cl_K of ideals of $\mathcal{O}_K$ modulo principal ideals and its *class number*$h_K = |\,\mathrm{Cl}_K\,|$ measure how far $\mathcal{O}_K$ is from behaving like $\mathbb{Z}$.

Using ideals introduces the additional difficulty of having to deal with $units$, the invertible elements of $\mathcal{O}_K$: Even when $h_K = 1$, a factorisation of ideals does not immediately yield a factorisation of numbers, since ideal generators are only defined up to units. For instance, the ideal factorisation $(6) = (2)\cdot(3)$ corresponds to the two factorisations $6 = 2\cdot 3$ and $6 = (-2)\cdot(-3)$. While in $\mathbb{Z}$, the only units are 1 and -1, the unit structure in general is that of a finitely generated $\mathbb{Z}$-module, whose generators are the *fundamental units*. The *regulator*R_K measures the "size" of the fundamental units as the volume of an associated lattice.

One of the main concerns of algorithmic algebraic number theory is to explicitly compute these invariants (Cl_K and h_K, fundamental units and R_K), as well as to provide the data allowing to efficiently compute with numbers and ideals of $\mathcal{O}_K$; see [28] for a recent account.

The *analytic class number formula* links the invariants h_K and R_K (unfortunately, only their product) to the ζ-function of K, $\zeta_K(s) := \prod_{\mathfrak{p} \text{ prime ideal of } \mathcal{O}_K} \left(1 - \mathrm{N}\,\mathfrak{p}^{-s}\right)^{-1}$, which is meaningful when $\Re(s) > 1$, but which may be extended to arbitrary complex $s \neq 1$. Introducing characters on the class group yields a generalisation of ζ- to L-functions. The *generalised Riemann hypothesis (GRH)*, which remains unproved even over the rationals, states that any such L-function does not vanish in the right half-plane $\Re(s) > 1/2$. The validity of the GRH has a dramatic impact on the performance of number theoretic algorithms. For instance, under GRH, the class group admits a system of generators of polynomial size; without GRH, only exponential bounds are known. Consequently, an algorithm to compute Cl_K via generators and relations (currently the only viable practical approach) either has to assume that GRH is true or immediately becomes exponential.

When $h_K = 1$ the number field K may be norm-Euclidean, endowing $\mathcal{O}_K$ with a Euclidean division algorithm. This question leads to the notions of the Euclidean minimum and spectrum of K, and another task in algorithmic number theory is to compute explicitly this minimum and the upper part of this spectrum, yielding for instance generalised Euclidean gcd algorithms.

3.2. Function fields, algebraic curves and cryptology

Participants: Karim Belabas, Guilhem Castagnos, Jean-Marc Couveignes, Andreas Enge, Enea Milio, Damien Robert, Emmanouil Tzortzakis.

Algebraic curves over finite fields are used to build the currently most competitive public key cryptosystems. Such a curve is given by a bivariate equation $\mathcal{C}(X,Y)=0$ with coefficients in a finite field $\mathbb{F}_q$. The main classes of curves that are interesting from a cryptographic perspective are *elliptic curves* of equation $\mathcal{C}=Y^2-(X^3+aX+b)$ and *hyperelliptic curves* of equation $\mathcal{C}=Y^2-(X^{2g+1}+\cdots)$ with $g\geqslant 2$.

The cryptosystem is implemented in an associated finite abelian group, the *Jacobian*$\mathrm{Jac}_{\mathcal{C}}$. Using the language of function fields exhibits a close analogy to the number fields discussed in the previous section. Let $\mathbb{F}_q(X)$ (the analogue of $\mathbb{Q}$) be the *rational function field* with subring $\mathbb{F}_q[X]$ (which is principal just as $\mathbb{Z}$). The *function field* of $\mathcal{C}$ is $K_{\mathcal{C}}=\mathbb{F}_q(X)[Y]/(\mathcal{C})$; it contains the *coordinate ring*$\mathcal{O}_{\mathcal{C}}=\mathbb{F}_q[X,Y]/(\mathcal{C})$. Definitions and properties carry over from the number field case $K/\mathbb{Q}$ to the function field extension $K_{\mathcal{C}}/\mathbb{F}_q(X)$. The Jacobian $\mathrm{Jac}_{\mathcal{C}}$ is the divisor class group of $K_{\mathcal{C}}$, which is an extension of (and for the curves used in cryptography usually equals) the ideal class group of $\mathcal{O}_{\mathcal{C}}$.

The size of the Jacobian group, the main security parameter of the cryptosystem, is given by an L-function. The GRH for function fields, which has been proved by Weil, yields the Hasse–Weil bound $(\sqrt{q}-1)^{2g}\leqslant|\,\mathrm{Jac}_{\mathcal{C}}\,|\leqslant(\sqrt{q}+1)^{2g}$, or $|\,\mathrm{Jac}_{\mathcal{C}}\,|\approx q^g$, where the *genus*$g$ is an invariant of the curve that correlates with the degree of its equation. For instance, the genus of an elliptic curve is 1, that of a hyperelliptic one is $\frac{\deg_X \mathcal{C}-1}{2}$. An important algorithmic question is to compute the exact cardinality of the Jacobian.

The security of the cryptosystem requires more precisely that the *discrete logarithm problem* (DLP) be difficult in the underlying group; that is, given elements D_1 and $D_2=xD_1$ of $\mathrm{Jac}_{\mathcal{C}}$, it must be difficult to determine x. Computing x corresponds in fact to computing $\mathrm{Jac}_{\mathcal{C}}$ explicitly with an isomorphism to an abstract product of finite cyclic groups; in this sense, the DLP amounts to computing the class group in the function field setting.

For any integer n, the *Weil pairing*e_n on $\mathcal{C}$ is a function that takes as input two elements of order n of $\mathrm{Jac}_{\mathcal{C}}$ and maps them into the multiplicative group of a finite field extension $\mathbb{F}_{q^k}$ with $k=k(n)$ depending on n. It is bilinear in both its arguments, which allows to transport the DLP from a curve into a finite field, where it is potentially easier to solve. The *Tate-Lichtenbaum pairing*, that is more difficult to define, but more efficient to implement, has similar properties. From a constructive point of view, the last few years have seen a wealth of cryptosystems with attractive novel properties relying on pairings.

For a random curve, the parameter k usually becomes so big that the result of a pairing cannot even be output any more. One of the major algorithmic problems related to pairings is thus the construction of curves with a given, smallish k.

3.3. Complex multiplication

Participants: Karim Belabas, Henri Cohen, Jean-Marc Couveignes, Andreas Enge, Fredrik Johansson, Chloë Martindale, Enea Milio, Damien Robert.

Complex multiplication provides a link between number fields and algebraic curves; for a concise introduction in the elliptic curve case, see [30], for more background material, [29]. In fact, for most curves $\mathcal{C}$ over a finite field, the endomorphism ring of $\mathrm{Jac}_{\mathcal{C}}$, which determines its L-function and thus its cardinality, is an order in a special kind of number field K, called *CM field*. The CM field of an elliptic curve is an imaginary-quadratic field $\mathbb{Q}(\sqrt{D})$ with $D<0$, that of a hyperelliptic curve of genus g is an imaginary-quadratic extension of a totally real number field of degree g. Deuring's lifting theorem ensures that $\mathcal{C}$ is the reduction modulo some prime of a curve with the same endomorphism ring, but defined over the *Hilbert class field*H_K of K.

Algebraically, H_K is defined as the maximal unramified abelian extension of K; the Galois group of H_K/K is then precisely the class group Cl_K. A number field extension H/K is called *Galois* if $H \simeq K[X]/(f)$ and H contains all complex roots of f. For instance, $\mathbb{Q}(\sqrt{2})$ is Galois since it contains not only $\sqrt{2}$, but also the second root $-\sqrt{2}$ of $X^2 - 2$, whereas $\mathbb{Q}(\sqrt[3]{2})$ is not Galois, since it does not contain the root $e^{2\pi i/3}\sqrt[3]{2}$ of $X^3 - 2$. The *Galois group*$\mathrm{Gal}_{H/K}$ is the group of automorphisms of H that fix K; it permutes the roots of f. Finally, an *abelian* extension is a Galois extension with abelian Galois group.

Analytically, in the elliptic case H_K may be obtained by adjoining to K the *singular value*$j(\tau)$ for a complex valued, so-called *modular* function j in some $\tau \in \mathcal{O}_K$; the correspondence between $\mathrm{Gal}_{H/K}$ and Cl_K allows to obtain the different roots of the minimal polynomial f of $j(\tau)$ and finally f itself. A similar, more involved construction can be used for hyperelliptic curves. This direct application of complex multiplication yields algebraic curves whose L-functions are known beforehand; in particular, it is the only possible way of obtaining ordinary curves for pairing-based cryptosystems.

The same theory can be used to develop algorithms that, given an arbitrary curve over a finite field, compute its L-function.

A generalisation is provided by *ray class fields*; these are still abelian, but allow for some well-controlled ramification. The tools for explicitly constructing such class fields are similar to those used for Hilbert class fields.

MARELLE Project-Team

3. Research Program

3.1. Type theory and formalization of mathematics

The calculus of inductive constructions is a branch of type theory that serves as a foundation for theorem proving tools, especially the Coq proof assistant. It is powerful enough to formalize complex mathematics, based on algebraic structures and operations. This is especially important as we want to produce proofs of logical properties for these algebraic structures, a goal that is only marginally addressed in most scientific computation systems.

The calculus of inductive constructions also makes it possible to write algorithms as recursive functional programs which manipulate tree-like data structures. A third important characteristic of this calculus is that it is also a language for manipulating proofs. All this makes this calculus a tool of choice for our investigations. However, this language still is the object of improvements and part of our work focusses on these improvements.

3.2. Verification of scientific algorithms

To produce certified algorithms, we use the following approach: instead of attempting to prove properties of an existing program written in a conventional programming language such as C or Java, we produce new programs in the calculus of constructions whose correctness is an immediate consequence of their construction. This has several advantages. First, we work at a high level of abstraction, independently of the target implementation language. Secondly, we concentrate on specific characteristics of the algorithm, and abstract away from the rest (for instance, we abstract away from memory management or data implementation strategies). Therefore, we are able to address more high-level mathematics and to express more general properties without being overwhelmed by implementation details.

However, this approach also presents a few drawbacks. For instance, the calculus of constructions usually imposes that recursive programs should explicitly terminate for all inputs. For some algorithms, we need to use advanced concepts (for instance, well-founded relations) to make the property of termination explicit, and proofs of correctness become especially difficult in this setting.

3.3. Programming language semantics

To bridge the gap between our high-level descriptions of algorithms and conventional programming languages, we investigate the algorithms that are present in programming language implementations, for instance algorithms that are used in a compiler or a static analysis tool. When working on these algorithms, we usually base our work on the semantic description of the programming language. The properties that we attempt to prove for an algorithm are, for example, that an optimization respects the meaning of programs or that the programs produced are free of some unwanted behavior. In practice, we rely on this study of programming language semantics to propose extensions to theorem proving tools or to verify that compilers for conventional programming languages are exempt from bugs.

MEXICO Project-Team

3. Research Program

3.1. Concurrency

Participants: Benedikt Bollig, Thomas Chatain, Paul Gastin, Stefan Haar, Serge Haddad, Stefan Schwoon.

Concurrency; Semantics; Automatic Control ; Diagnosis ; Verification

Concurrency: Property of systems allowing some interacting processes to be executed in parallel.

Diagnosis: The process of deducing from a partial observation of a system aspects of the internal states or events of that system; in particular, *fault diagnosis* aims at determining whether or not some non-observable fault event has occurred.

Conformance Testing: Feeding dedicated input into an implemented system IS and deducing, from the resulting output of I, whether I respects a formal specification S.

3.1.1. Introduction

It is well known that, whatever the intended form of analysis or control, a *global* view of the system state leads to overwhelming numbers of states and transitions, thus slowing down algorithms that need to explore the state space. Worse yet, it often blurs the mechanics that are at work rather than exhibiting them. Conversely, respecting concurrency relations avoids exhaustive enumeration of interleavings. It allows us to focus on 'essential' properties of non-sequential processes, which are expressible with causal precedence relations. These precedence relations are usually called causal (partial) orders. Concurrency is the explicit absence of such a precedence between actions that do not have to wait for one another. Both causal orders and concurrency are in fact essential elements of a specification. This is especially true when the specification is constructed in a distributed and modular way. Making these ordering relations explicit requires to leave the framework of state/interleaving based semantics. Therefore, we need to develop new dedicated algorithms for tasks such as conformance testing, fault diagnosis, or control for distributed discrete systems. Existing solutions for these problems often rely on centralized sequential models which do not scale up well.

3.1.2. Diagnosis

Participants: Benedikt Bollig, Stefan Haar, Serge Haddad, Stefan Schwoon.

Fault Diagnosis for discrete event systems is a crucial task in automatic control. Our focus is on *event oriented* (as opposed to *state oriented*) model-based diagnosis, asking e.g. the following questions:
given a - potentially large - *alarm pattern* formed of observations,

- what are the possible *fault scenarios* in the system that *explain* the pattern ?
- Based on the observations, can we deduce whether or not a certain - invisible - fault has actually occurred ?

Model-based diagnosis starts from a discrete event model of the observed system - or rather, its relevant aspects, such as possible fault propagations, abstracting away other dimensions. From this model, an extraction or unfolding process, guided by the observation, produces recursively the explanation candidates.

In asynchronous partial-order based diagnosis with Petri nets [51], [52], [56], one unfolds the *labelled product* of a Petri net model $\mathcal{N}$ and an observed alarm pattern $\mathcal{A}$, also in Petri net form. We obtain an acyclic net giving partial order representation of the behaviors compatible with the alarm pattern. A recursive online procedure filters out those runs *(configurations)* that explain *exactly*$\mathcal{A}$. The Petri-net based approach generalizes to dynamically evolving topologies, in dynamical systems modeled by graph grammars, see [35]

3.1.2.1. Observability and Diagnosability

Diagnosis algorithms have to operate in contexts with low observability, i.e., in systems where many events are invisible to the supervisor. Checking *observability* and *diagnosability* for the supervised systems is therefore a crucial and non-trivial task in its own right. Analysis of the relational structure of occurrence nets allows us to check whether the system exhibits sufficient visibility to allow diagnosis. Developing efficient methods for both verification of *diagnosability checking* under concurrency, and the *diagnosis* itself for distributed, composite and asynchronous systems, is an important field for *MExICo*.

3.1.2.2. Distribution

Distributed computation of unfoldings allows one to factor the unfolding of the global system into smaller *local* unfoldings, by local supervisors associated with sub-networks and communicating among each other. In [52], [37], elements of a methodology for distributed computation of unfoldings between several supervisors, underwritten by algebraic properties of the category of Petri nets have been developed. Generalizations, in particular to Graph Grammars, are still do be done.

Computing diagnosis in a distributed way is only one aspect of a much vaster topic, that of *distributed diagnosis* (see [48], [60]). In fact, it involves a more abstract and often indirect reasoning to conclude whether or not some given invisible fault has occurred. Combination of local scenarios is in general not sufficient: the global system may have behaviors that do not reveal themselves as faulty (or, dually, non-faulty) on any local supervisor's domain (compare [34], [40]). Rather, the local diagnosers have to join all *information* that is available to them locally, and then deduce collectively further information from the combination of their views. In particular, even the *absence* of fault evidence on all peers may allow to deduce fault occurrence jointly, see [64], [65]. Automatizing such procedures for the supervision and management of distributed and locally monitored asynchronous systems is a long-term goal to which *MExICo* hopes to contribute.

3.1.3. Contextual nets

Participant: Stefan Schwoon.

Assuring the correctness of concurrent systems is notoriously difficult due to the many unforeseeable ways in which the components may interact and the resulting state-space explosion. A well-established approach to alleviate this problem is to model concurrent systems as Petri nets and analyse their unfoldings, essentially an acyclic version of the Petri net whose simpler structure permits easier analysis [50].

However, Petri nets are inadequate to model concurrent read accesses to the same resource. Such situations often arise naturally, for instance in concurrent databases or in asynchronous circuits. The encoding tricks typically used to model these cases in Petri nets make the unfolding technique inefficient. Contextual nets, which explicitly do model concurrent read accesses, address this problem. Their accurate representation of concurrency makes contextual unfoldings up to exponentially smaller in certain situations. An abstract algorithm for contextual unfoldings was first given in [36]. In recent work, we further studied this subject from a theoretical and practical perspective, allowing us to develop concrete, efficient data structures and algorithms and a tool (Cunf) that improves upon existing state of the art. This work led to the PhD thesis of César Rodríguez in 2014 .

Contexutal unfoldings deal well with two sources of state-space explosion: concurrency and shared resources. Recently, we proposed an improved data structure, called *contextual merged processes* (CMP) to deal with a third source of state-space explosion, i.e. sequences of choices. The work on CMP [66] is currently at an abstract level. In the short term, we want to put this work into practice, requiring some theoretical groundwork, as well as programming and experimentation.

Another well-known approach to verifying concurrent systems is *partial-order reduction*, exemplified by the tool SPIN. Although it is known that both partial-order reduction and unfoldings have their respective strengths and weaknesses, we are not aware of any conclusive comparison between the two techniques. Spin comes with a high-level modeling language having an explicit notion of processes, communication channels, and variables. Indeed, the reduction techniques implemented in Spin exploit the specific properties of these features. On the other side, while there exist highly efficient tools for unfoldings, Petri nets are a relatively general low-level formalism, so these techniques do not exploit properties of higher language features. Our work on contextual unfoldings and CMPs represents a first step to make unfoldings exploit richer models. In the long run, we wish raise the unfolding technique to a suitable high-level modelling language and develop appropriate tool support.

3.1.4. Dynamic and parameterized concurrent systems

Participants: Benedikt Bollig, Paul Gastin.

In the past few years, our research has focused on concurrent systems where the architecture, which provides a set of processes and links between them, is *static* and *fixed in advance*. However, the assumption that the set of processes is fixed somehow seems to hinder the application of formal methods in practice. It is not appropriate in areas such as mobile computing or ad-hoc networks. In concurrent programming, it is actually perfectly natural to design a program, and claim its correctness, independently of the number of processes that participate in its execution. There are, essentially, two kinds of systems that fall into this category. When the process architecture is static but unknown, it is a parameter of the system; we then call a system *parameterized*. When, on the other hand, the process architecure is generated at runtime (i.e., process creation is a communication primitive), we say that a system is *dynamic*. Though parameterized and dynamic systems have received increasing interest in recent years, there is, by now, no canonical approach to modeling and verifying such systems. Our research program aims at the development of *a theory of parameterized and dynamic concurrent systems*. More precisely, our goal is a *unifying* theory that lays algebraic, logical, and automata-theoretic foundations to support and facilitate the study of parameterized and dynamic concurrent systems. Such theories indeed exist in non-parameterized settings where the number of processes and the way they are connected are fixed in advance. However, parameterized and dynamic systems lack such foundations and often restict to very particular models with specialized verification techniques.

3.1.5. Testing

Participants: Benedikt Bollig, Paul Gastin, Stefan Haar.

3.1.5.1. Introduction

The gap between specification and implementation is at the heart of research on formal testing. The general *conformance testing problem* can be defined as follows: Does an implementation $\mathcal{M}'$ conform a given specification $\mathcal{M}$? Here, both $\mathcal{M}$ and $\mathcal{M}'$ are assumed to have input and output channels. The formal model $\mathcal{M}$ of the specification is entirely known and can be used for analysis. On the other hand, the implementation $\mathcal{M}'$ is unknown but interacts with the environment through observable input and output channels. So the behavior of $\mathcal{M}'$ is partially controlled by input streams, and partially observable via output streams. The Testing problem consists in computing, from the knowledge of $\mathcal{M}$, *input streams* for $\mathcal{M}'$ such that observation of the resulting output streams from $\mathcal{M}'$ allows to determine whether $\mathcal{M}'$ conforms to $\mathcal{M}$ as intended.

In this project, we focus on distributed or asynchronous versions of the conformance testing problem. There are two main difficulties. First, due to the distributed nature of the system, it may not be possible to have a unique global observer for the outcome of a test. Hence, we may need to use *local* observers which will record only *partial views* of the execution. Due to this, it is difficult or even impossible to reconstruct a coherent global execution. The second difficulty is the lack of global synchronization in distributed asynchronous systems. Up to now, models were described with I/O automata having a centralized control, hence inducing global synchronizations.

3.1.5.2. Asynchronous Testing

Since 2006 and in particular during his sabbatical stay at the University of Ottawa, Stefan Haar has been working with Guy-Vincent Jourdan and Gregor v. Bochmann of UOttawa and Claude Jard of IRISA on asynchronous testing. In the synchronous (sequential) approach, the model is described by an I/O automaton with a centralized control and transitions labeled with individual input or output actions. This approach has known limitations when inputs and outputs are distributed over remote sites, a feature that is characteristic of , e.g., web computing. To account for concurrency in the system, they have developed in [58], [41] asynchronous conformance testing for automata with transitions labeled with (finite) partial orders of I/O. Intuitively, this is a "big step" semantics where each step allows concurrency but the system is synchronized before the next big step. This is already an important improvement on the synchronous setting. The non-trivial challenge is now to cope with fully asynchronous specifications using models with decentralized control such as Petri nets.

3.1.5.3. Near Future

Completion of asynchronous testing in the setting without any big-step synchronization, and an improved understanding of the relations and possible interconnections between local (i.e. distributed) and asynchronous (centralized) testing. This has been the objective of the *TECSTES* project (2011-2014), funded by a DIGITEO *DIM/LSC* grant, and which involved Hernán Ponce de Léon and Stefan Haar of *MExICo*, and Delphine Longuet at LRI, University Paris-Sud/Orsay. We have extended several well known conformance (ioco style) relations for sequential models to models that can handle concurrency (labeled event structures). Two semantics (interleaving and partial order) were presented for every relation. With the interleaving semantics, the relations we obtained boil down to the same relations defined for labeled transition systems, since they focus on sequences of actions. The only advantage of using labeled event structures as a specification formalism for testing remains in the conciseness of the concurrent model with respect to a sequential one. As far as testing is concerned, the benefit is low since every interleaving has to be tested. By contrast, under the partial order semantics, the relations we obtain allow to distinguish explicitly implementations where concurrent actions are implemented concurrently, from those where they are interleaved, i.e. implemented sequentially. Therefore, these relations will be of interest when designing distributed systems, since the natural concurrency between actions that are performed in parallel by different processes can be taken into account. In particular, the fact of being unable to control or observe the order between actions taking place on different processes will not be considered as an impediment for testing. We have developped a complete testing framework for concurrent systems, which included the notions of test suites and test cases. We studied what kind of systems are testable in such a framework, and we have proposed sufficient conditions for obtaining a complete test suite as well as an algorithm to construct a test suite with such properties.

A mid-to long term goal (which may or may not be addressed by *MExICo* depending on the availability of staff for this subject) is the comprehensive formalization of testing and testability in asynchronous systems with distributed architecture and test protocols.

3.2. Interaction

Participants: Benedikt Bollig, Thomas Chatain, Paul Gastin, Stefan Haar, Serge Haddad.

3.2.1. Introduction

Systems and services exhibit non-trivial *interaction* between specialized and heterogeneous components. This interplay is challenging for several reasons. On one hand, a coordinated interplay of several components is required, though each has only a limited, partial view of the system's configuration. We refer to this problem as *distributed synthesis* or *distributed control*. An aggravating factor is that the structure of a component might be semi-transparent, which requires a form of *grey box management*.

Interaction, one of the main characteristics of systems under consideration, often involves an environment that is not under the control of cooperating services. To achieve a common goal, the services need to agree upon a strategy that allows them to react appropriately regardless of the interactions with the environment. Clearly, the notions of opponents and strategies fall within *game theory*, which is naturally one of our main tools in exploring interaction. We will apply to our problems techniques and results developed in the domains of distributed games and of games with partial information. We will consider also new problems on games that arise from our applications.

3.2.2. Distributed Control

Participants: Benedikt Bollig, Thomas Chatain, Paul Gastin, Stefan Haar.

Program synthesis, as introduced by Church [47] aims at deriving directly an implementation from a specification, allowing the implementation to be correct by design. When the implementation is already at hand but choices remain to be resolved at run time then the problem becomes controller synthesis. Both program and controller synthesis have been extensively studied for sequential systems. In a distributed setting, we need to synthesize a distributed program or distributed controllers that interact locally with the system components. The main difficulty comes from the fact that the local controllers/programs have only a partial view of the entire system. This is also an old problem largely considered undecidable in most settings [63], [59], [62], [53], [55].

Actually, the main undecidability sources come from the fact that this problem was addressed in a synchronous setting using global runs viewed as sequences. In a truly distributed system where interactions are asynchronous we have recently obtained encouraging decidability results [54], [45]. This is a clear witness where concurrency may be exploited to obtain positive results. It is essential to specify expected properties directly in terms of causality revealed by partial order models of executions (MSCs or Mazurkiewicz traces). We intend to develop this line of research with the ambitious aim to obtain decidability for all natural systems and specifications. More precisely, we will identify natural hypotheses both on the architecture of our distributed system and on the specifications under which the distributed program/controller synthesis problem is decidable. This should open the way to important applications, e.g., for distributed control of embedded systems.

3.2.3. Adaptation and Grey box management

Participants: Stefan Haar, Serge Haddad.

Contrary to mainframe systems or monolithic applications of the past, we are experiencing and using an increasing number of services that are performed not by one provider but rather by the interaction and cooperation of many specialized components. As these components come from different providers, one can no longer assume all of their internal technologies to be known (as it is the case with proprietary technology). Thus, in order to compose e.g. orchestrated services over the web, to determine violations of specifications or contracts, to adapt existing services to new situations etc, one needs to analyze the interaction behavior of *boxes* that are known only through their public interfaces. For their semi-transparent-semi-opaque nature, we shall refer to them as **grey boxes**. While the concrete nature of these boxes can range from vehicles in a highway section to hotel reservation systems, the tasks of *grey box management* have universal features allowing for generalized approaches with formal methods. Two central issues emerge:

- Abstraction: From the designer point of view, there is a need for a trade-off between transparency (no abstraction) in order to integrate the box in different contexts and opacity (full abstraction) for security reasons.
- Adaptation: Since a grey box gives a partial view about the behavior of the component, even if it is not immediately useable in some context, the design of an adaptator is possible. Thus the goal is the synthesis of such an adaptator from a formal specification of the component and the environment.

Our work on direct modeling and handling of "grey boxes" via modal models (see [49]) was halted when Dorsaf El-Hog stopped her PhD work to leave academia, and has not resumed for lack of staff. However, it should be noted that semi-transparent system management in a larger sense remains an active field for the team, witness in particular our work on diagnosis and testing.

3.3. Management of Quantitative Behavior

Participants: Benedikt Bollig, Thomas Chatain, Paul Gastin, Stefan Haar, Serge Haddad.

3.3.1. Introduction

Besides the logical functionalities of programs, the *quantitative* aspects of component behavior and interaction play an increasingly important role.

- *Real-time* properties cannot be neglected even if time is not an explicit functional issue, since transmission delays, parallelism, etc, can lead to time-outs striking, and thus change even the logical course of processes. Again, this phenomenon arises in telecommunications and web services, but also in transport systems.
- In the same contexts, *probabilities* need to be taken into account, for many diverse reasons such as unpredictable functionalities, or because the outcome of a computation may be governed by race conditions.
- Last but not least, constraints on *cost* cannot be ignored, be it in terms of money or any other limited resource, such as memory space or available CPU time.

Traditional mainframe systems were proprietary and (essentially) localized; therefore, impact of delays, unforeseen failures, etc. could be considered under the control of the system manager. It was therefore natural, in verification and control of systems, to focus on *functional* behavior entirely.

With the increase in size of computing system and the growing degree of compositionality and distribution, quantitative factors enter the stage:

- calling remote services and transmitting data over the web creates *delays*;
- remote or non-proprietary components are not “deterministic”, in the sense that their behavior is uncertain.

Time and *probability* are thus parameters that management of distributed systems must be able to handle; along with both, the *cost* of operations is often subject to restrictions, or its minimization is at least desired. The mathematical treatment of these features in distributed systems is an important challenge, which *MExICo* is addressing; the following describes our activities concerning probabilistic and timed systems. Note that cost optimization is not a current activity but enters the picture in several intended activities.

3.3.2. Probabilistic distributed Systems

Participants: Stefan Haar, Serge Haddad, Claudine Picaronny.

3.3.2.1. Non-sequential probabilistic processes

Practical fault diagnosis requires to select explanations of *maximal likelihood*. For partial-order based diagnosis, this leads therefore to the question what the probability of a given partially ordered execution is. In Benveniste et al. [39], [32], we presented a model of stochastic processes, whose trajectories are partially ordered, based on local branching in Petri net unfoldings; an alternative and complementary model based on Markov fields is developed in [57], which takes a different view on the semantics and overcomes the first model’s restrictions on applicability.

Both approaches abstract away from real time progress and randomize choices in *logical* time. On the other hand, the relative speed - and thus, indirectly, the real-time behavior of the system’s local processes - are crucial factors determining the outcome of probabilistic choices, even if non-determinism is absent from the system.

In another line of research [43] we have studied the likelihood of occurrence of non-sequential runs under random durations in a stochastic Petri net setting. It remains to better understand the properties of the probability measures thus obtained, to relate them with the models in logical time, and exploit them e.g. in *diagnosis*.

3.3.2.2. Distributed Markov Decision Processes

Participant: Serge Haddad.

Distributed systems featuring non-deterministic and probabilistic aspects are usually hard to analyze and, more specifically, to optimize. Furthermore, high complexity theoretical lower bounds have been established for models like partially observed Markovian decision processes and distributed partially observed Markovian decision processes. We believe that these negative results are consequences of the choice of the models rather than the intrinsic complexity of problems to be solved. Thus we plan to introduce new models in which the associated optimization problems can be solved in a more efficient way. More precisely, we start by studying connection protocols weighted by costs and we look for online and offline strategies for optimizing the mean cost to achieve the protocol. We have been cooperating on this subject with the SUMO team at Inria Rennes; in the joint work [33]; there, we strive to synthesize for a given MDP a control so as to guarantee a specific stationary behavior, rather than - as is usually done - so as to maximize some reward.

3.3.3. Large scale probabilistic systems

Addressing large-scale probabilistic systems requires to face state explosion, due to both the discrete part and the probabilistic part of the model. In order to deal with such systems, different approaches have been proposed:

- Restricting the synchronization between the components as in queuing networks allows to express the steady-state distribution of the model by an analytical formula called a product-form [38].
- Some methods that tackle with the combinatory explosion for discrete-event systems can be generalized to stochastic systems using an appropriate theory. For instance symmetry based methods have been generalized to stochastic systems with the help of aggregation theory [46].
- At last simulation, which works as soon as a stochastic operational semantic is defined, has been adapted to perform statistical model checking. Roughly speaking, it consists to produce a confidence interval for the probability that a random path fulfills a formula of some temporal logic [67] .

We want to contribute to these three axes: (1) we are looking for product-forms related to systems where synchronization are more involved (like in Petri nets), see [2]; (2) we want to adapt methods for discrete-event systems that require some theoretical developments in the stochastic framework and, (3) we plan to address some important limitations of statistical model checking like the expressiveness of the associated logic and the handling of rare events.

3.3.4. Real time distributed systems

Nowadays, software systems largely depend on complex timing constraints and usually consist of many interacting local components. Among them, railway crossings, traffic control units, mobile phones, computer servers, and many more safety-critical systems are subject to particular quality standards. It is therefore becoming increasingly important to look at networks of timed systems, which allow real-time systems to operate in a distributed manner.

Timed automata are a well-studied formalism to describe reactive systems that come with timing constraints. For modeling distributed real-time systems, networks of timed automata have been considered, where the local clocks of the processes usually evolve at the same rate [61] [44]. It is, however, not always adequate to assume that distributed components of a system obey a global time. Actually, there is generally no reason to assume that different timed systems in the networks refer to the same time or evolve at the same rate. Any component is rather determined by local influences such as temperature and workload.

3.3.4.1. Implementation of Real-Time Concurrent Systems

Participants: Thomas Chatain, Stefan Haar, Serge Haddad.

This was one of the tasks of the ANR ImpRo.

Formal models for real-time systems, like timed automata and time Petri nets, have been extensively studied and have proved their interest for the verification of real-time systems. On the other hand, the question of using these models as specifications for designing real-time systems raises some difficulties. One of those comes from the fact that the real-time constraints introduce some artifacts and because of them some syntactically correct models have a formal semantics that is clearly unrealistic. One famous situation is the case of Zeno executions, where the formal semantics allows the system to do infinitely many actions in finite time. But there are other problems, and some of them are related to the distributed nature of the system. These are the ones we address here.

One approach to implementability problems is to formalize either syntactical or behavioral requirements about what should be considered as a reasonable model, and reject other models. Another approach is to adapt the formal semantics such that only realistic behaviors are considered.

These techniques are preliminaries for dealing with the problem of implementability of models. Indeed implementing a model may be possible at the cost of some transformation, which make it suitable for the target device. By the way these transformations may be of interest for the designer who can now use high-level features in a model of a system or protocol, and rely on the transformation to make it implementable.

We aim at formalizing and automating translations that preserve both the timed semantics and the concurrent semantics. This effort is crucial for extending concurrency-oriented methods for logical time, in particular for exploiting partial order properties. In fact, validation and management - in a broad sense - of distributed systems is not realistic *in general* without understanding and control of their real-time dependent features; the link between real-time and logical-time behaviors is thus crucial for many aspects of *MExICo*'s work.

3.3.5. Weighted Automata and Weighted Logics

Participants: Benedikt Bollig, Paul Gastin.

Time and probability are only two facets of quantitative phenomena. A generic concept of adding weights to qualitative systems is provided by the theory of weighted automata [31]. They allow one to treat probabilistic or also reward models in a unified framework. Unlike finite automata, which are based on the Boolean semiring, weighted automata build on more general structures such as the natural or real numbers (equipped with the usual addition and multiplication) or the probabilistic semiring. Hence, a weighted automaton associates with any possible behavior a weight beyond the usual Boolean classification of “acceptance” or “non-acceptance”. Automata with weights have produced a well-established theory and come, e.g., with a characterization in terms of rational expressions, which generalizes the famous theorem of Kleene in the unweighted setting. Equipped with a solid theoretical basis, weighted automata finally found their way into numerous application areas such as natural language processing and speech recognition, or digital image compression.

What is still missing in the theory of weighted automata are satisfactory connections with verification-related issues such as (temporal) logic and bisimulation that could lead to a general approach to corresponding satisfiability and model-checking problems. A first step towards a more satisfactory theory of weighted systems was done in [42]. That paper, however, does not give definite answers to all the aforementioned problems. It identifies directions for future research that we will be tackling.

MUTANT Project-Team

3. Research Program

3.1. Machine Listening

Participants: Arshia Cont, Philippe Cuvillier, Florent Jacquemard, Maxime Sirbu, Adrien Ycart.

When human listeners are confronted with musical sounds, they rapidly and automatically find their way in the music. Even musically untrained listeners have an exceptional ability to make rapid judgments about music from short examples, such as determining music style, performer, beating, and specific events such as instruments or pitches. Making computer systems capable of similar capabilities requires advances in both music cognition, and analysis and retrieval systems employing signal processing and machine learning.

Machine listening in our context refers to the capacity of our computers to understand "non-speech sound" by analyzing the content of music and audio signals and combining advanced signal processing and machine learning. The major focus of MuTant has been on Real-time Machine listening algorithms spanning *Real-time Recognition Systems* (such as event detection) and also *Information Retrieval* (such as structure discovery and qualitative parameter estimation). Our major achievement lies in our unique Real-time Score Following (aka Audio-to-Score Alignment) system that are featured in the Antescofo system (cf. Section 5.1). We also contributed to the field of On-line Music Structure Discovery in Audio Processing, and lately to the problem of off-line rhythmic quantization on Symbolic Data.

3.1.1. Real-time Audio-to-Score Alignment.

This is a continuation of prior work of team-founder [1] which proved the utility of strongly-timed probabilistic models in form of Semi-Markov Hidden States. Our most important theoretical contribution is reported in [37], [38] that introduced Time-coherency criteria for probabilistic models and led to general robustness of the Antescofo listening machine, and allowed its deployment for all music instruments and all setups around the world. We further studied the integration of other recognition algorithms in the algorithm in form of *Information Fusion* and for singing voice based on Lyric data in [49]. Collaboration with our japanese counterparts led to extensions of our model to the symbolic domain reported in [56]. Collaboration with the SIERRA team created a joint research momentum for fostering such applications to weakly-supervised discriminative models reported in [54]. Our Real-time Audio-to-Score alignment is a major component of the Antescofo software described in Section 5.1 .

3.1.2. Online Methods for Audio Segmentation and Clustering.

To extend our listening approach to general sound, we envisioned dropping the prior information provided by music scores and replacing it by the inherent structure in general audio signals. Early attempts by the team leader employed [2] Methods of Information Geometry, an attempt to join Information Theory, Differential Geometry and Signal Processing. We were among the first teams in the world advocating the use of such approaches for audio signal processing and we participated in the growth of the community. A major breakthrough of this approach is reported in [39] and the PhD Thesis [40] that outline a general real-time change detection mechanism. Automatic structure discovery was further pursued in a MS thesis project in 2013 [55]. By that time we realized that Information Manifolds do not necessarily provide the invariance needed for automatic structure discovery of audio signals, especially for natural sounds. Following this report, we pursued an alternative approach in 2014 and in collaboration with the Inria SIERRA Team [30]. The result of this joint work was published in IEEE ICASSP 2015 and won the best student paper award [29]. We are currently studying massive applications of this approach to natural sounds and in robotics applications in the framework of Maxime Sirbu's PhD project.

3.1.3. Symbolic Music Information Retrieval and Rhythm Transcription.

Rhythmic data are commonly represented by tree structures (rhythms trees) due to the theoretical proximity of such structures with the proportional representation of time values in traditional musical notation. We are studying the application to rhythm notation of techniques and tools for symbolic processing of tree structures, in particular tree automata and term rewriting.

Our main contribution in that context is the development of a new framework for rhythm transcription [23], [22], [65], [31] addressing the problem of converting a sequence of timestamped notes, *e.g.* a file in MIDI format, into a score in traditional music notation. This problem is crucial in the context assisted music composition environments and music score editors. It arises immediately as insoluble unequivocally: in order to fit the musical context, the system has to balance constraints of precision and readability of the generated scores. Our approach is based on algorithms for the exploration and lazy enumeration of large sets of weighted trees (tree series), representing possible solutions to a problem of transcription. A side problem concerns the equivalent notations of the same rhythm, for which we have developed a term rewrite approach, based on a new equational theory of rhythm notation [42], [51], [52].

3.2. Synchronous and realtime programming for computer music

Participants: Julia Blondeau, Arshia Cont, Jean-Louis Giavitto.

The research presented here aims at the development of a programming model dedicated to authoring of time and interaction for the next generation of interactive music systems. Study, formalization and implementation of such programming paradigm, strongly coupled to recognition systems discussed in the previous section, constitutes the second objective of the MuTant project.

The tangible result of this research is the development of the Antescofo system (cf. Section 5.1) for the design and implementation of musical scenarios in which the human and computer actions are in constant real-time interaction. Through such development, Antescofo has already made itself into the community; it serves as the backbone of temporal organization of more than 100 performances since 2012 and used both for preexisting pieces and new creations by music ensembles such as Berliner Philharmoniker, Los Angeles Philharmonic, Ensemble Intercontemporain or Orchestre de Paris to name a few.

Compared to programmable sequencers or interactive music systems (like Max or PureData) the Antescofo DSL offers a rich notion of time reference and provides explicit time frame for the environment with a comprehensive list of musical synchronization strategies and proposes and predictable mechanisms for controlling time at various timescales (temporal determinism) and across concurrent code modules (time-mediated concurrency).

3.2.1. Multiple Times.

Audio and music often involve the presence and cooperation of multiple notions of *time*: an ideal time authored by the composer in a score and also a performance time produced jointly by the performers and the real-time electronics; where instant and duration are expressed both in physical time (milliseconds), in relative time (relative to an unknown dynamic tempo) or through logical events and relations (“at the peak of intensity”, “at the end of the musical phrase”, “twice faster”).

Antescofo is the first languages that addresses this variety of temporal notions, relying on the synchronous approach for the handling of atomic and logical events and an anticipative notion of tempo for the handling of relative duration [35], [45]. A first partial model of time at work in Antescofo (single time, static activities) has been formalized relying on parametric timed automata [43] and constitutes the reference semantics for tests (cf. section 3.3). A denotational semantics of the complete language (multiple times and dynamic constructions including anticipative synchronization strategies) has been published in [44].

3.2.2. Human-Computer Synchronizations.

Antescofo introduces the notion of *temporal scope* to formalize relationships between temporal information specified in the score and their realization during a performance [36]. A temporal scope is attached to a sequence of actions, can be inherited or dynamically changed as a result of a computation. A synchronization strategy is part of a temporal scope definition. They use the performer's position information and its tempo estimation from the listening module, to drive the passing of time in a sequence of atomic and durative actions.

Synchronization strategies have been systematically studied to evaluate their musical relevance in collaboration with Orchestre de Paris and composer Marco Stroppa. Anticipative strategies enable handling of uncertainties inherent in musical event occurrence, exhibiting a smooth musical rendering whilst preserving articulation points and target events [63].

3.2.3. Temporal Organization.

Several constructions dedicated to the expression of the temporal organization of musical entities and their control have enriched the language from the start of the project. These construction have been motivated by composer's research residences in our team: representation of open scores (J. Freeman); anticipative synchronization strategies (C. Trapani); adaptive sampling of continuous curve in relative time for the dynamic control of sound synthesis (J.-M. Fernandez); musical gesture (J. Blondeau); first class processes, actors and continuation combinators for the development of libraries of reusable parametric temporal behaviors (M. Stroppa, Y. Maresz); *etc.*

The reaction to a logical event is a unique feature in the computer music system community [57]. It extend the well known `when` operator in synchronous languages with process creation. Elaborating on this low-level mechanism, *temporal patterns* [48] enable expression of complex temporal constraints mixing instant and duration. The problem of online matching where the event are presented in real time and the matching is computed incrementally as well, has received a recent attention from the model-checking community, but with less constrained causal constraints.

3.2.4. Visualization and Monitoring of Event-driven and Time-driven Computations.

The authoring of complex temporal organization can be greatly improved through adapted visual interfaces, and has led to the development of *AscoGraph*, a dedicated user interface to Antescofo. Ascograph is used both for edition and monitoring interface of the system during performances [34]. This project was held from end 2012 to end 2014 thanks to Inria ADT and ANR support.

An information visualisation perspective has been taken for the design of timeline-based representation of action items, looking for information coherence and clarity, facility of seeking and navigation, hierarchical distinction and explicit linking [33] while minimizing the information overload for the presentation of the nested structure of complex concurrent activities [32].

3.3. Semantics, Verification and Test of Mixed Scores

Participants: Jean-Louis Giavitto, Florent Jacquemard, Clément Poncelet.

We address the questions of *functional reliability* and *temporal predictability* in score-based interactive music systems such as Antescofo. On the one hand, checking these properties is difficult for these systems involving an amount of human interactions as well as timing constraints (for audio computations) beyond those of many other real-time applications such as embedded control. On the other hand, although they are expected to behave properly during public concerts, these systems are not safety critical, and therefore a complete formal certification is not strictly necessary in our case.

Our objective in this context is to provide techniques and tools to assist both programmers of scores (*i.e.* composers) and the developers of the system itself. [47], [46]. It should be outlined that the former are generally not experts in real-time programming, and we aim at giving them a clear view of what will be the outcome of the score that they are writing, and what are the limits of what is playable by the system. To help the development of Antescofo, we have built a framework for automated timed conformance testing. [14], [18], [58], [60], [59].

In both cases, it is important to be able to predict statically the behavior of the system in response to every possible musician input. This cannot be done manually and requires first a formal definition of the semantics of scores, and second using advanced symbolic state exploration techniques (model checking) [43].

PACAP Project-Team

3. Research Program

3.1. Motivation

Our research program is naturally driven by the evolution of our ecosystem. Relevant recent changes can be classified in the following categories: technological constraints, evolving community, and domain constraints. We hereby summarize these evolutions.

3.1.1. Technological constraints

Until recently, binary compatibility guaranteed portability of programs, while increased clock frequency and improved micro-architecture provided increased performance. However, in the last decade, advances in technology and micro-architecture started translating into more parallelism instead. Technology roadmaps even predict the feasibility of thousands of cores on a chip by 2020. Hundreds are already commercially available. Since the vast majority of applications are still sequential, or contain significant sequential sections, such a trend put an end to the automatic performance improvement enjoyed by developers and users. Many research groups consequently focused on parallel architectures and compiling for parallelism.

The focus of ALF – and the DAL ERC – was paradoxically on Amdahl's law: the performance of applications will ultimately be driven by the performance of the sequential part. Despite a number of advances (some of them contributed by ALF), sequential tasks are still a major performance bottleneck. Addressing it is still on the agenda of the proposed PACAP project-team.

In addition, due to power constraints, only part of the billions of transistors of a microprocessor can be operated at any given time (the *dark silicon* paradigm). A sensible approach consists in specializing parts of the silicon area to provide dedicated accelerators (not run simultaneously). This results in diverse and heterogeneous processor cores. Application and compiler designers are now confronted with a moving target, challenging portability and jeopardizing performance.

Finally, we live in a world where billions of sensors, actuators, and computers play a crucial role in our life: flight control, nuclear plant management, defense systems, banking, or health care. These systems must be reliable, despite the fact that they are subject to faults (for example due to aging, charged particle hit, or random noise). Faults will soon become the new *de facto* standard. The evolutions of the semiconductor industry predict an exponential growth of the number of permanent faults [58]. Reliability considerations usually degrade performance. We will propose solutions to mitigate this impact (for example by limiting overheads to critical sections).

Note on technology.
Technology also progresses at a fast pace. We do not propose to pursue any research on technology *per se*. Recently proposed paradigms (quantum computing, non-Si, brain-inspired) have received lots of attention from the research community. We do *not* intend to invest in those paradigms, but we will continue to investigate compilation and architecture for more conventional programming paradigms. Still, several technological shifts may have consequences for us, and we will closely monitor their developments, they include for example non-volatile memory (impacts security, makes writes longer than loads), 3D-stacking (impacts bandwidth), and photonics (impacts latencies and connection network).

3.1.2. Evolving community

The PACAP project-team will tackle performance-related issues, for conventional programming paradigms. In fact, programming complex environments is no longer reserved to experts in compilation and architecture. A large community now develops applications for a wide range of targets, including mobile “apps”, cloud, multicore or heterogeneous processors.

This also includes domain scientists (in biology, medicine, but also social sciences) who started relying heavily on computational resources, gathering huge amounts of data, and requiring considerable amount of processing to analyze them. Our research is motivated by the growing discrepancy between on the one hand the complexity of the workloads and the computing systems, and on the other hand the expanding community of developers at large, with limited expertise to optimize and to map efficiently computations to compute nodes.

3.1.3. Domain constraints

Mobile, embedded systems have become ubiquitous. Many of them have real-time constraints. For this class of systems, correctness implies not only producing the correct result, but also doing so within specified deadlines. In the presence of heterogeneous, complex and highly dynamic systems, producing *tight* (i.e. useful) upper bound to the worst-case execution time has become extremely challenging. Our research will aim at improving the tightness as well as enlarging the set of features that can be safely analyzed.

The ever growing dependence of our economy on computing systems also implies that security has become of utmost importance. Many systems are under constant attacks from intruders. Protection has a cost also in terms of performance. We plan to leverage our background to contribute solutions that minimize this impact.

Note on Applications Domains.
As was already the case for ALF, PACAP will work on fundamental technologies for computer science: processor architecture, performance-oriented compilation and guaranteed response time for real-time. The research results may have impacts on any application domain that requires high performance execution (telecommunication, multimedia, biology, health, engineering, environment...), but also on many embedded applications that exhibit other constraints such as power consumption, code size and guaranteed response time.

We strive to extract from active domains the fundamental characteristics that are relevant to our research. For example, *big data* is of interest to PACAP because it relates to the study of hardware/software mechanisms to efficiently transfer huge amounts of data to the computing nodes. Similarly, the *Internet of Things* is of interest because it has implications in terms of ultra low power consumption.

3.2. Research Objectives

Processor micro-architecture and compilation have been at the core of the research carried by the CAPS and ALF project teams for two decades, with undeniable contributions. They will continue to be the foundation of PACAP.

Heterogeneity and diversity of processor architectures now require new techniques to guarantee that the hardware is satisfactorily exploited by the software. We will devise new static compilation techniques (cf. Section 3.2.1), but also build upon iterative [1] and split [2] compilation to continuously adapt software to its environment (Section 3.2.2). Dynamic binary optimization will also play a key role in delivering adapting software and delivering performance.

The end of Moore's law and Dennard's scaling [0] offer an exciting window of opportunity, where performance improvements will no longer derive from additional transistor budget or increased clock frequency, but rather come from breakthroughs in microarchitecture (Section 3.2.3). We will also consider how to reconcile CPU and GPU designs (Section 3.2.4).

Heterogeneity and multicores are also major obstacles to determining tight worst-case execution times of real-time systems (Section 3.2.5), which we plan to tackle.

Finally, we also describe how we plan to address transversal aspects such reliability (Section 3.2.6), power efficiency (Section 3.2.7), and security (Section 3.2.8).

[0] According to Dennard scaling, as transistors get smaller the power density remains constant, and the consumed power remains proportional to the area.

3.2.1. Static Compilation

Static compilation techniques will continue to be relevant to address the characteristics of emerging hardware technologies, such as non-volatile memories, 3D-stacking, or novel communication technologies. These techniques expose new characteristics to the software layers. As an example, non-volatile memories typically have asymmetric read-write latencies (writes are much longer than reads) and different power consumption profiles. PACAP will study the new optimization opportunities and develop tailored compilation techniques for the upcoming compute nodes. New technologies may also be coupled with traditional solutions to offer new trade-offs. We will study how programs can adequately exploit the specific features of the proposed heterogeneous compute nodes.

We propose to build upon iterative compilation [1] to explore how applications perform on different configurations. When possible, Pareto points will be related to application characteristics. The best configuration, however, may actually depend on runtime information, such as input data, dynamic events, or properties that are available only at runtime. Unfortunately a runtime system has little time and means to determine the best configuration. For these reasons, we will also leverage split-compilation [2]: the idea consists in pre-computing alternatives, and embedding in the program enough information to assist and drive a runtime system towards to the best solution.

3.2.2. Software Adaptation

More than ever, software will need to adapt to their environment. In most cases, this environment will remain unknown until runtime. This is already the case when one deploys an application to a cloud, or an “app” to mobile devices. The dilemma is the following: for maximum portability, developers should target the most general device; but for performance they would like to exploit the most recent and advanced hardware features. JIT compilers can handle the situation to some extent, but binary deployment requires dynamic binary rewriting. Our work has shown how SIMD instructions can be upgraded from SSE to AVX [3]. Many more opportunities will appear with diverse and heterogeneous processors, featuring various kinds of accelerators.

On shared hardware, the environment is also defined by other applications competing for the same computational resources. It will become increasingly important to adapt to changing runtime conditions, such as the contention of the cache memories, available bandwidth, or hardware faults. Fortunately, optimizing at runtime is also an opportunity, because this is the first time the program is visible as a whole: executable and libraries (including library versions). Optimizers may also rely on dynamic information, such as actual input data, parameter values, etc. We have already developed a software platform [14] to analyze and optimize programs at runtime, and we started working on automatic dynamic parallelization of sequential code, and dynamic specialization.

We started addressing some of these challenges in ongoing projects such as Nano2017 PSAIC Collaborative research program with STMicroelectronics, as well as within the Inria Project Lab MULTICORE. The starting H2020 FET HPC project ANTAREX will also address these challenges from the energy perspective. We will further leverage our platform and initial results to address other adaptation opportunities. Efficient software adaptation will require expertise from all domains tackled by PACAP, and strong interaction between all team members is expected.

3.2.3. Research directions in uniprocessor microarchitecture

Achieving high single-thread performance remains a major challenge even in the multicore era (Amdahl’s law). The members of the PACAP project-team have been conducting research in uniprocessor microarchitecture research for about 20 years covering major topics including caches, instruction front-end, branch prediction, out-of-order core pipeline, branch prediction and value prediction. In particular, in the recent years they have been recognized world leaders in branch prediction [19][9] and in cache prefetching [7] and they have revived the forgotten concept of value prediction [12], [11]. This research was supported by the ERC Advanced grant DAL (2011-2016) and also by Intel. We intend to pursue research on achieving ultimate unicore performance. Below are several non-orthogonal directions that we have identified for midterm research:

1. management of the memory hierarchy (particularly the hardware prefetching);
2. practical design of very wide issue execution core;
3. speculative execution.

Memory design issues:
Performance of many applications is highly impacted by the memory hierarchy behavior. The interactions between the different components in the memory hierarchy and the out-of-order execution engine have high impact on performance.

The last *Data Prefetching Contest* held with ISCA 2015 has illustrated that achieving high prefetching efficiency is still a challenge for wide-issue superscalar processors, particularly those featuring a very large instruction window. The large instruction window enables an implicit data prefetcher. The interaction between this implicit hardware prefetcher and the explicit hardware prefetcher is still relatively mysterious as illustrated by Pierre Michaud's BO prefetcher (winner of DPC2) [7]. The first objective of the research is to better understand how the implicit prefetching enabled by the large instruction window interacts with the L2 prefetcher and then to understand how explicit prefetching on the L1 also interacts with the L2 prefetcher.

The second objective of the research is related to the interaction of prefetching and virtual/physical memory. On real hardware, prefetching is stopped by page frontiers. The interaction between TLB prefetching (and on which level) and cache prefetching must be analyzed.

The prefetcher is not the only actor in the hierarchy that must be carefully controlled. Significant benefit can also be achieved through careful management of memory access bandwidth, particularly the management of spatial locality on memory accesses, both for reads and writes. The exploitation of this locality is traditionally handled in the memory controller. However, it could be better handled if larger temporal granularity was available. Finally, we also intend to continue to explore the promising avenue of compressed caches. In particular we recently proposed the skewed compressed cache [15]. It offers new possibility for efficient compression schemes.

Ultra wide-issue superscalar.
To effectively leverage memory level parallelism, one requires huge out-of-order execution structures as well as very wide issue superscalar processor. For the two past decades, implementing always wider issue superscalar processor has been challenging. The objective of our research on the execution core is to explore (and revisit) directions to allow the design of a very wide-issue (8-to-16 way) out-of-order execution core while mastering its complexity (silicon area, hardware logic complexity, power/energy consumption).

The first direction that we intend to explore is the use of clustered architecture as in our recent work [8]. Symmetric clustered organization allows to benefit from simpler bypass network, but induce large complexity on the issue queue. One remarkable finding of our study [8] is that, when considering two large clusters (e.g. 8-wide) steering large groups of consecutive instructions (e.g. 64 μops) to the same cluster is quite efficient. This opens opportunities to limit the complexity of the issue queues (monitoring less fewer buses) and register files (reducing number of ports, and number of physical registers) in the clusters, since not all results have to be forwarded to the other cluster.

The second direction that we intend to explore is associated with the approach we developed with Sembrant et al. [16]. It reduces the number of instructions waiting in the instruction queues for the applications benefiting from very large instruction windows. Instructions are dynamically classified as ready (independent from any long latency instruction) or non-ready, and as urgent (part of a dependency chain leading to a long latency instruction) or non-urgent. Non-ready non-urgent instructions can be delayed until the long latency instruction has been executed; this allows to reduce the pressure on the issue queue. This proposition opens the opportunity to consider an asymmetric microarchitecture with a cluster dedicated to the execution of urgent instructions and a second cluster executing the non-urgent instructions. The microarchitecture of this second cluster could be optimized to reduce complexity and power consumption (smaller instruction queue, less aggressive scheduling...)

Speculative execution.

Out-of-order (OoO) execution relies on speculative execution that requires predictions of all sorts: branch, memory dependency, value...

The PACAP members have been major actors of the branch prediction research for the last 20 years; and their proposals have influenced the design of most of the hardware branch predictors in current microprocessors. We will continue to steadily explore new branch predictor designs as for instance [18].

In speculative execution, we have recently revisited value prediction (VP) which was a hot research topic between 1996 and 2002. However it was considered up to recently that value prediction would lead to a huge increase in complexity and power consumption in every stage of the pipeline. Fortunately, we have recently shown that complexity usually introduced by value prediction in the OoO engine can be overcome [12], [11], [19], [9]. First, very high accuracy can be enforced at reasonable cost in coverage and minimal complexity [12]. Thus, both prediction validation and recovery by squashing can be done outside the out-of-order engine, at commit time. Furthermore, we propose a new pipeline organization, EOLE ({Early | Out-of-order | Late} Execution), that leverages VP with validation at commit to execute many instructions outside the OoO core, in-order [11]. With EOLE, the issue-width in OoO core can be reduced without sacrificing performance, thus benefiting the performance of VP without a significant cost in silicon area and/or energy. In the near future, we will explore new avenues related to value prediction. These directions include register equality prediction and compatibility of value prediction with weak memory models in multiprocessors.

3.2.4. Towards heterogeneous single-ISA CPU-GPU architectures

Heterogeneous single-ISA architectures have been proposed in the literature during the 2000's [56] and are now widely used in the industry (ARM big.LITTLE, NVIDIA 4+1...) as a way to improve power-efficiency in mobile processors. These architectures include multiple cores whose respective microarchitectures offer different trade-offs between performance and energy efficiency, or between latency and throughput, while offering the same interface to software. Dynamic task migration policies leverage the heterogeneity of the platform by using the most suitable core for each application, or even each phase of processing. However, these works only tune cores by changing their complexity. Energy-optimized cores are either identical cores implemented in a low-power process technology, or simplified in-order superscalar cores, which are far from state-of-the-art throughput-oriented architectures such as GPUs.

We propose to investigate the convergence of CPU and GPU at both architecture and compilation levels.

Architecture.
The architecture convergence between Single Instruction Multiple Threads (SIMT) GPUs and multicore processors that we have been pursuing [36] opens the way for heterogeneous architectures including latency-optimized superscalar cores and throughput-optimized GPU-style cores, which all share the same instruction set. Using SIMT cores in place of superscalar cores will enable the highest energy efficiency on regular sections of applications. As with existing single-ISA heterogeneous architectures, task migration will not necessitate any software rewrite and will accelerate existing applications.

Compilers for emerging heterogeneous architectures.
Single-ISA CPU+GPU architectures will provide the necessary substrate to enable efficient heterogeneous processing. However, it will also introduce substantial challenges at the software and firmware level. Task placement and migration will require advanced policies that leverage both static information at compile time and dynamic information at run-time. We are tackling the heterogeneous task scheduling problem at the compiler level. As a first step, we are prototyping scheduling algorithms on existing multiple-ISA CPU+GPU architectures like NVIDIA Tegra X1.

3.2.5. Real-time systems

Safety-critical systems (e.g. avionics, medical devices, automotive...) have so far used simple unicore hardware systems as a way to control their predictability, in order to meet timing constraints. Still, many critical embedded systems have increasing demand in computing power, and simple unicore processors are not sufficient anymore. General-purpose multicore processors are not suitable for safety-critical real-time systems, because they include complex micro-architectural elements (cache hierarchies, branch, stride and value predictors) meant to improve average-case performance, and for which worst-case performance is difficult to predict. The prerequisite for calculating tight WCET is a deterministic hardware system that avoids dynamic, time-unpredictable calculations at run-time.

Even for multi and manycore systems designed with time-predictability in mind (Kalray MPPA manycore architecture [0], or the Recore manycore hardware [0]) calculating WCETs is still challenging. The following two challenges will be addressed in the mid-term:

1. definition of methods to estimate WCETs tightly on manycores, that smartly analyzes and/or controls shared resources such as buses, NoCs or caches;
2. methods to improve the programmability of real-time applications through automatic parallelization and optimizations from model-based designs.

3.2.6. Fault Tolerance

Technology trends suggest that, in tomorrow's computing world, failures will become commonplace due to many factors, and the expected probability of failure will increase with scaling. While well-known approaches, such as error correcting codes, exist to recover from failures and provide fault-free chips, the exponential growth of the number of faults will make them unaffordable in the future. Consequently, other approaches such as fine-grained disabling and reconfiguration of hardware elements (e.g. individual functional units or cache blocks) will become economically necessary. We are going to enter a new era: functionally correct chips with variable performance among chips and throughout their lifetime [58].

Transient and permanent faults may be detected by similar techniques, but correcting them generally involves different approaches. We are primarily interested in permanent faults, even though we do not necessarily disregard transient faults (e.g. the TMR approach in the next paragraph addresses both kind of faults).

CPU.
Permanent faults can occur anywhere in the processor. The performance implications of faulty cells vary depending on how the array is used in a processor. Most of micro-architectural work aiming at assessing the performance implications of permanently faulty cells relies on simulations with random fault-maps. These studies are, therefore, limited by the fault-maps they use that may not be representative for the average and distributed performance. They also do not consider aging effect.

Considering the memory hierarchy, we have already studied [5] the impact of permanent faults on the average and worst-case performance based on analytical models. We will extend these models to cover other components and other designs, and to analyze the interaction between faulty components.

For identified critical hardware structures, such as the memory hierarchy, we will propose protection mechanisms by for instance using larger cells, or even by selecting a different array organization to mitigate the impact of faults.

Another approach to deal with faults is to introduce redundancy at the code level. We propose to consider static compilation techniques focusing on existing hardware. As an example, we plan to leverage SIMD extensions of current instruction sets to introduce redundancy in scalar code at minimum cost. With these instructions, it will be possible to protect the execution from both soft errors by using TMR (triple modular redundancy) with voters in the code itself, and permanent faults without the need of extra hardware support to deconfigure faulty functional units.

Reconfigurable Computing.

[0] http://www.kalrayinc.com
[0] http://www.recoresystems.com/

In collaboration with the CAIRN project-team, we propose to construct Coarse Grain Reconfigurable Architectures (CGRA) from a sea of basic arithmetic and memory elements organized into clusters and connected through a hierarchical interconnection network. These clusters of basic arithmetic operators (e.g. 8-bit arithmetic and logic units) would be able to be seamlessly configured to various accuracy and data types to adapt the consumed energy to application requirements taking advantage of approximate computations. We propose to add new kinds of error detection (and sometimes correction) directly at the operator level by taking advantage of the massive redundancy of the array. As an example, errors can be tracked and detected in a complex sequence of double floating-point operations by using a reduced-precision version of the same processing.

Such reconfigurable blocks will be driven by compilation techniques, in charge of computing checkpoints, detecting faults, and replaying computations when needed.

Dynamic compilation techniques will help better exploit faulty hardware, by allocating data and computations on correct resources. In case of permanent faults, we will provide a mechanism to reconfigure the hardware, for example by reducing the issue width of VLIW processors implemented in CGRA. Dynamic code generation (JIT compiler) will re-generate code for the new configuration, guaranteeing portability and optimal exploitation of the hardware.

3.2.7. Power efficiency

PACAP will address power-efficiency at several levels. First, we will design static and split compilation techniques to contribute to the race for Exascale computing (the general goal is to reach 10^{18} FLOP/s at less than 20 MW). Second, we will focus on high-performance low-power embedded compute nodes. will research new static and dynamic compilation techniques that fully exploit emerging memory and NoC technologies. Finally, in collaboration with the CAIRN project-team, we will investigate the synergy of reconfigurable computing and dynamic code generation.

Green and heterogeneous high-performance computing.
Concerning HPC systems, our approach consists in mapping, runtime managing and autotuning applications for green and heterogeneous High-Performance Computing systems up to the Exascale level. One key innovation of the proposed approach consists of introducing a separation of concerns (where self-adaptivity and energy efficient strategies are specified aside to application functionalities) promoted by the definition of a Domain Specific Language (DSL) inspired by aspect-oriented programming concepts for heterogeneous systems. The new DSL will be introduced for expressing adaptivity/energy/performance strategies and to enforce at runtime application autotuning and resource and power management. The goal is to support the parallelism, scalability and adaptability of a dynamic workload by exploiting the full system capabilities (including energy management) for emerging large-scale and extreme-scale systems, while reducing the Total Cost of Ownership (TCO) for companies and public organizations.

High-performance low-power embedded compute nodes.
We will address the design of next generation energy-efficient high-performance embedded compute nodes. It focuses at the same time on software, architecture and emerging memory and communication technologies in order to synergistically exploit their corresponding features. The approach of the project is organized around three complementary topics: 1) compilation techniques; 2) multicore architectures; 3) emerging memory and communication technologies. PACAP will focus on the compilation aspects, taking as input the software-visible characteristics of the proposed emerging technology, and making the best possible use of the new features (non-volatility, density, endurance, low-power).

Hardware Accelerated JIT Compilation.
Reconfigurable hardware offers the opportunity to limit power consumption by dynamically adjusting the number of available resources to the requirements of the running software. In particular, VLIW processors can adjust the number of available issue lanes. Unfortunately, changing the processor width often requires recompiling the application, and VLIW processors are highly dependent of the quality of the compilation, mainly because of the instruction scheduling phase performed by the compiler. Another challenge lies in the high constraints of the embedded system: the energy and execution time overhead due to the JIT compilation must be carefully kept under control.

We started exploring ways to reduce the cost of JIT compilation targeting VLIW-based heterogeneous many-core systems. Our approach lies on a hardware/software JIT compiler framework. While basic optimizations and JIT management are performed in software, the compilation back-end is implemented by means of specialized hardware. This back-end involves both instruction scheduling and register allocation, which are known to be the most time-consuming stages of such a compiler.

3.2.8. Security

Security is a mandatory concern of any modern computing system. Various threat models have led to a multitude of protection solutions. ALF already has contributions, thanks to the HAVEGE [62] random number generator, and code obfuscating techniques (the obfuscating just-in-time compiler [55], or thread-based control flow mangling [60]).

We plan to partner with security experts who can provide intuition, know-how and expertise, in particular in defining threat models, and assessing the quality of the solutions. Our background in compilation and architecture will help design more efficient and less expensive protection mechanisms.

We already have ongoing research directions related to security. We also plan to partner with the Inria/CentraleSupelec CIDRE project-team to design a tainting technique based on a just-in-time compiler.

Compiler-based data protection.
We will specify and design error correction codes suitable for an efficient protection of sensitive information in the context of Internet of Things (IoT) and connected objects. We will partner with experts in security and codes to prototype a platform that demonstrates resilient software. PACAP's expertise will be key to select and tune the protection mechanisms developed within the project, and to propose safe, yet cost-effective solutions from an implementation point of view.

JIT-based tainting.
Dynamic information flow control (DIFC, also known as *tainting*) is used used to detect intrusions and to identify vulnerabilities. It consists in attaching metadata (called *taints* or *labels*) to information containers, and to propagate the taints when particular operations are applied to the containers: reads, writes, etc. The goal is then to guarantee that confidential information is never used to generate data sent to an untrusted container; conversely, data produced by untrusted entities cannot be used to update sensitive data.

The containers can be of various granularities: fine-grain approaches can deal with single variables, coarser-grain approaches consider a file as a whole. The CIDRE project-team has developed several DIFC monitors. kBlare is coarse-grain monitor in the Linux kernel. JBlare is a fine-grain monitor for Java applications. Fine-grain monitors provide a better precision at the cost of a significant overhead in execution time.

We propose to combine the expertise of CIDRE in DIFC with our expertise in JIT compilation to design hybrid approaches. An initial static analysis of the program prior to installation or execution will feed information to a dynamic analyzer that propagates taints during just-in-time compilation.

PARKAS Project-Team

3. Research Program

3.1. Programming Languages for Cyber-Physical Systems

We study the definition of languages for reactive and Cyber-Physical Systems in which distributed control software interacts closely with physical devices. We focus on languages that mix discrete-time and continuous-time; in particular, the combination of synchronous programming constructs with differential equations, relaxed models of synchrony for distributed systems communicating via periodic sampling or through buffers, and the embedding of synchronous features in a general purpose ML language.

The synchronous language SCADE, [0] based on synchronous languages principles, is ideal for programming embedded software and is used routinely in the most critical applications. But embedded design also involves modeling the control software together with its environment made of physical devices that are traditionally defined by differential equations that evolve on a continuous-time basis and approximated with a numerical solver. Furthermore, compilation usually produces single-loop code, but implementations increasingly involve multiple and multi-core processors communicating via buffers and shared-memory.

The major player in embedded design for cyber-physical systems is undoubtedly SIMULINK, [0] with MODELICA[0] a new player. Models created in these tools are used not only for simulation, but also for test-case generation, formal verification, and translation to embedded code. That said, many foundational and practical aspects are not well-treated by existing theory (for instance, hybrid automata), and current tools. In particular, features that mix discrete and continuous time often suffer from inadequacies and bugs. This results in a broken development chain: for the most critical applications, the model of the controller must be reprogrammed into either sequential or synchronous code, and properties verified on the source model have to be reverified on the target code. There is also the question of how much confidence can be placed in the code used for simulation.

We attack these issues through the development of the ZELUS research prototype, industrial collaborations with the SCADE team at ANSYS/Esterel-Technologies, and collaboration with Modelica developers at Dassault-Systèmes and the Modelica association. Our approach is to develop a *conservative extension* of a synchronous language capable of expressing in a single source text a model of the control software and its physical environment, to simulate the whole using off-the-shelf numerical solvers, and to generate target embedded code. Our goal is to increase faithfulness and confidence in both what is actually executed on platforms and what is simulated. The goal of building a language on a strong mathematical basis for hybrid systems is shared with the Ptolemy project at UC Berkeley; our approach is distinguished by building our language on a synchronous semantics, reusing and extending classical synchronous compilation techniques.

Adding continuous time to a synchronous language gives a richer programming model where reactive controllers can be specified in idealized physical time. An example is the so called quasi-periodic architecture studied by Caspi, where independent processors execute periodically and communicate by sampling. We have applied ZELUS to model a class of quasi-periodic protocols and to analyze an abstraction proposed for model-checking such systems.

Communication-by-sampling is suitable for control applications where value timeliness is paramount and lost or duplicate values tolerable, but other applications—for instance, those involving video streams—seek a different trade-off through the use of bounded buffers between processes. We developed the *n*-synchronous model and the programming language LUCY-N to treat this issue.

[0] http://www.esterel-technologies.com/products/scade-suite

[0] http://www.mathworks.com/products/simulink

[0] https://www.modelica.org

3.2. Efficient Compilation for Parallel and Distributed Computing

We develop compilation techniques for sequential and multi-core processors, and efficient parallel run-time systems for computationally intensive real-time applications (e.g., video and streaming). We study the generation of parallel code from synchronous programs, compilation techniques based on the polyhedral model, and the exploitation of synchronous Single Static Assignment (SSA) representations in general purpose compilers.

We consider distribution and parallelism as two distinct concepts.

- Distribution refers to the construction of multiple programs which are dedicated to run on specific computing devices. When an application is designed for, or adapted to, an embedded multiprocessor, the distribution task grants fine grained—design- or compilation-time—control over the mapping and interaction between the multiple programs.
- Parallelism is about generating code capable of efficiently exploiting multiprocessors. Typically this amounts to maing (in)dependence properties, data transfers, atomicity and isolation explicit. Compiling parallelism translates these properties into low-level synchronization and communication primitives and/or onto a runtime system.

We also see a strong relation between the foundations of synchronous languages and the design of compiler intermediate representations for concurrent programs. These representations are essential to the construction of compilers enabling the optimization of parallel programs and the management of massively parallel resources. Polyhedral compilation is one of the most popular research avenues in this area. Indirectly, the design of intermediate representations also triggers exciting research on dedicated runtime systems supporting parallel constructs. We are particularly interested in the implementation of non-blocking dynamic schedulers interacting with decoupled, deterministic communication channels to hide communication latency and optimize local memory usage.

While distribution and parallelism issues arise in all areas of computing, our programming language perspective pushes us to consider four scenarios:

1. designing an embedded system, both hardware and software, and codesign;
2. programming existing embedded hardware with functional and behavioral constraints;
3. programming and compiling for a general-purpose or high-performance, best-effort system;
4. programming large scale distributed, I/O-dominated and data-centric systems.

We work on a multitude of research experiments, algorithms and prototypes related to one or more of these scenarios. Our main efforts focused on extending the code generation algorithms for synchronous languages and on the development of more scalable and widely applicable polyhedral compilation methods.

3.3. Validation and Proof of Compilers

Compilers are complex software and not immune from bugs. We work on validation and proof tools for compilers to relate the semantics of executed code and source programs. We develop techniques to formally prove the correctness of compilation passes for synchronous languages (Lustre), and to validate compilation optimization for C code in the presence of threads.

3.3.1. Lustre:

The formal validation of a compiler for a synchronous language (or more generally for a language based on synchronous block diagrams) promises to reduce the likelihood of compiler-introduced bugs, the cost of testing, and also to ensure that properties verified on the source model hold of the target code. Such a validation would be complementary to existing industrial qualifications which certify the development process and not the functional correctness of a compiler. The scientific interest is in developing models and techniques that both facilitate the verification and allow for convenient reasoning over the semantics of a language and the behavior of programs written in it.

3.3.2. C/C++:

The recently approved C11 and C++11 standards define a concurrency model for the C and C++ languages, which were originally designed without concurrency support. Their intent is to permit most compiler and hardware optimizations, while providing escape mechanisms for writing portable, high-performance, low-level code. Mainstream compilers are being modified to support the new standards. A subtle class of compiler bugs is the so-called concurrency compiler bugs, where compilers generate correct sequential code but break the concurrency memory model of the programming language. Such bugs are observable only when the miscompiled functions interact with concurrent contexts, making them particularly hard to detect. All previous techniques to test compiler correctness miss concurrency compiler bugs.

PARSIFAL Project-Team

3. Research Program

3.1. General overview

There are two broad approaches for computational specifications. In the *computation as model* approach, computations are encoded as mathematical structures containing nodes, transitions, and state. Logic is used to *describe* these structures, that is, the computations are used as models for logical expressions. Intensional operators, such as the modals of temporal and dynamic logics or the triples of Hoare logic, are often employed to express propositions about the change in state.

The *computation as deduction* approach, in contrast, expresses computations logically, using formulas, terms, types, and proofs as computational elements. Unlike the model approach, general logical apparatus such as cut-elimination or automated deduction becomes directly applicable as tools for defining, analyzing, and animating computations. Indeed, we can identify two main aspects of logical specifications that have been very fruitful:

- *Proof normalization*, which treats the state of a computation as a proof term and computation as normalization of the proof terms. General reduction principles such as β-reduction or cut-elimination are merely particular forms of proof normalization. Functional programming is based on normalization [69], and normalization in different logics can justify the design of new and different functional programming languages [41].
- *Proof search*, which views the state of a computation as a a structured collection of formulas, known as a *sequent*, and proof search in a suitable sequent calculus as encoding the dynamics of the computation. Logic programming is based on proof search [75], and different proof search strategies can be used to justify the design of new and different logic programming languages [73].

While the distinction between these two aspects is somewhat informal, it helps to identify and classify different concerns that arise in computational semantics. For instance, confluence and termination of reductions are crucial considerations for normalization, while unification and strategies are important for search. A key challenge of computational logic is to find means of uniting or reorganizing these apparently disjoint concerns.

An important organizational principle is structural proof theory, that is, the study of proofs as syntactic, algebraic and combinatorial objects. Formal proofs often have equivalences in their syntactic representations, leading to an important research question about *canonicity* in proofs – when are two proofs “essentially the same?” The syntactic equivalences can be used to derive normal forms for proofs that illuminate not only the proofs of a given formula, but also its entire proof search space. The celebrated *focusing* theorem of Andreoli [43] identifies one such normal form for derivations in the sequent calculus that has many important consequences both for search and for computation. The combinatorial structure of proofs can be further explored with the use of *deep inference*; in particular, deep inference allows access to simple and manifestly correct cut-elimination procedures with precise complexity bounds.

Type theory is another important organizational principle, but most popular type systems are generally designed for either search or for normalization. To give some examples, the Coq system [85] that implements the Calculus of Inductive Constructions (CIC) is designed to facilitate the expression of computational features of proofs directly as executable functional programs, but general proof search techniques for Coq are rather primitive. In contrast, the Twelf system [80] that is based on the LF type theory (a subsystem of the CIC), is based on relational specifications in canonical form (*i.e.*, without redexes) for which there are sophisticated automated reasoning systems such as meta-theoretic analysis tools, logic programming engines, and inductive theorem provers. In recent years, there has been a push towards combining search and normalization in the same type-theoretic framework. The Beluga system [81], for example, is an extension of the LF type theory with a purely computational meta-framework where operations on inductively defined LF objects can be expressed as functional programs.

The Parsifal team investigates both the search and the normalization aspects of computational specifications using the concepts, results, and insights from proof theory and type theory.

3.2. Inductive and co-inductive reasoning

The team has spent a number of years in designing a strong new logic that can be used to reason (inductively and co-inductively) on syntactic expressions containing bindings. This work is based on earlier work by McDowell, Miller, and Tiu [71] [70] [76] [86], and on more recent work by Gacek, Miller, and Nadathur [4] [56]. The Parsifal team, along with our colleagues in Minneapolis, Canberra, Singapore, and Cachen, have been building two tools that exploit the novel features of this logic. These two systems are the following.

- Abella, which is an interactive theorem prover for the full logic.
- Bedwyr, which is a model checker for the "finite" part of the logic.

We have used these systems to provide formalize reasoning of a number of complex formal systems, ranging from programming languages to the λ-calculus and π-calculus.

Since 2014, the Abella system has been extended with a number of new features. A number of new significant examples have been implemented in Abella and an extensive tutorial for it has been written [1].

3.3. Developing a foundational approach to defining proof evidence

The team is developing a framework for defining the semantics of proof evidence. With this framework, implementers of theorem provers can output proof evidence in a format of their choice: they will only need to be able to formally define that evidence's semantics. With such semantics provided, proof checkers can then check alleged proofs for correctness. Thus, anyone who needs to trust proofs from various provers can put their energies into designing trustworthy checkers that can execute the semantic specification.

In order to provide our framework with the flexibility that this ambitious plan requires, we have based our design on the most recent advances within the theory of proofs. For a number of years, various team members have been contributing to the design and theory of *focused proof systems* [45] [48] [49] [50] [59] [67] [68] and we have adopted such proof systems as the corner stone for our framework.

We have also been working for a number of years on the implementation of computational logic systems, involving, for example, both unification and backtracking search. As a result, we are also building an early and reference implementation of our semantic definitions.

3.4. Deep inference

Deep inference [61], [63] is a novel methodology for presenting deductive systems. Unlike traditional formalisms like the sequent calculus, it allows rewriting of formulas deep inside arbitrary contexts. The new freedom for designing inference rules creates a richer proof theory. For example, for systems using deep inference, we have a greater variety of normal forms for proofs than in sequent calculus or natural deduction systems. Another advantage of deep inference systems is the close relationship to categorical proof theory. Due to the deep inference design one can directly read off the morphism from the derivations. There is no need for a counter-intuitive translation.

The following research problems are investigated by members of the Parsifal team:

- Find deep inference system for richer logics. This is necessary for making the proof theoretic results of deep inference accessible to applications as they are described in the previous sections of this report.
- Investigate the possibility of focusing proofs in deep inference. As described before, focusing is a way to reduce the non-determinism in proof search. However, it is well investigated only for the sequent calculus. In order to apply deep inference in proof search, we need to develop a theory of focusing for deep inference.

3.5. Proof nets and atomic flows

Proof nets and atomic flows are abstract (graph-like) presentations of proofs such that all "trivial rule permutations" are quotiented away. Ideally the notion of proof net should be independent from any syntactic formalism, but most notions of proof nets proposed in the past were formulated in terms of their relation to the sequent calculus. Consequently we could observe features like “boxes” and explicit “contraction links”. The latter appeared not only in Girard’s proof nets [58] for linear logic but also in Robinson’s proof nets [83] for classical logic. In this kind of proof nets every link in the net corresponds to a rule application in the sequent calculus.

Only recently, due to the rise of deep inference, new kinds of proof nets have been introduced that take the formula trees of the conclusions and add additional “flow-graph” information (see e.g., [6], [5] and [62]. On one side, this gives new insights in the essence of proofs and their normalization. But on the other side, all the known correctness criteria are no longer available.

This directly leads to the following research questions investigated by members of the Parsifal team:

- Finding (for classical logic) a notion of proof nets that is deductive, i.e., can effectively be used for doing proof search. An important property of deductive proof nets must be that the correctness can be checked in linear time. For the classical logic proof nets by Lamarche and Straßburger [6] this takes exponential time (in the size of the net).
- Studying the normalization of proofs in classical logic using atomic flows. Although there is no correctness criterion they allow to simplify the normalization procedure for proofs in deep inference, and additionally allow to get new insights in the complexity of the normalization.

3.6. Cost Models and Abstract Machines for Functional Programs

In the *proof normalization* approach, computation is usually reformulated as the evaluation of functional programs, expressed as terms in a variation over the λ-calculus. Thanks to its higher-order nature, this approach provides very concise and abstract specifications. Its strength is however also its weakness: the abstraction from physical machines is pushed to a level where it is no longer clear how to measure the complexity of an algorithm.

Models like Turing machines or RAM rely on atomic computational steps and thus admit quite obvious cost models for time and space. The λ-calculus instead relies on a single non-atomic operation, β-reduction, for which costs in terms of time and space are far from evident.

Nonetheless, it turns out that the number of β-steps is a reasonable time cost model, i.e.,it is polynomially related to those of Turing machines and RAM. For the special case of *weak evaluation* (i.e., reducing only β-steps that are not under abstractions)—which is used to model functional programming languages—this is a relatively old result due to Blelloch and Greiner [46] (1995). It is only very recently (2014) that the strong case—used in the implementation models of proof assistants—has been solved by Accattoli and Dal Lago [42].

With the recent recruitment of Accattoli, the team’s research has expanded in this direction. The topics under investigations are:

1. *Complexity of Abstract Machines*. Bounding and comparing the overhead of different abstract machines for different evaluation schemas (weak/strong call-by-name/value/need λ-calculi) with respect to the cost model. The aim is the development of a complexity-aware theory of the implementation of functional programs.
2. *Reasonable Space Cost Models*. Essentially nothing is known about reasonable space cost models. It is known, however, that environment-based execution model—which are the mainstream technology for functional programs—do not provide an answer. We are exploring the use of the non-standard implementation models provided by Girard’s Geometry of Interaction to address this question.

PESTO Project-Team

3. Research Program

3.1. Modelling

Before being able to analyse and properly design security protocols, it is essential to have a model with a precise semantics of the protocols themselves, the attacker and its capabilities, as well as the properties a protocol needs to ensure.

Most current languages for protocol specification are quite basic and do not provide support for global state, loops, or complex data structures such as lists, or Merkle trees. As an example we may cite Hardware Security Modules that rely on a notion of *mutable global state* which does not arise in traditional protocols, see e.g. the discussion by Herzog [46].

Similarly, the properties a protocol should satisfy are generally not precisely defined, and stating the "right" definitions is often a challenging task in itself. In the case of authentication, many protocol attacks were due to the lack of a precise meaning, cf [44]. While the case of authentication has been widely studied, the recent digitalisation of all kinds of transactions and services, introduces a plethora of new properties, including for instance anonymity in e-voting, untraceability of RFID tokens, verifiability of computations that are outsourced, as well as sanitisation of data in social networks. We expect that many privacy anonymity properties may be modelled as particular observational equivalences in process calculi [40], or indistinguishability between cryptographic games [2], sanitisation of data may also rely on information-theoretic measures.

We also need to take into account that the attacker model changes. While historically the attacker was considered to control the communication network, we may nowadays argue that even (part of) the host executing the software may be compromised through, e.g., malware. This situation motivates the use of secure elements and multi-factor authentication with out-of-band channels. A typical example occurs in e-commerce: to validate an online payment a user needs to enter an additional code sent by the bank via sms to the user's mobile phone. Such protocols require the possession of a physical device in addition to the knowledge of a password which could have been leaked on an untrusted platform. The fact that data needs to be copied by a human requires these data to be *short*, and hence amenable to brute-force attacks by an attacker or guessing.

3.2. Analysis

3.2.1. Generic proof techniques

Most automated tools for verifying security properties rely on techniques stemming from automated deduction. Often existing techniques do however not apply directly, or do not scale up due to the state explosion problems. For instance, the use of Horn clause resolution techniques requires dedicated resolution methods [34][3]. Another example is unification modulo equational theory, which is a key technique in several tools, e.g. [43]. Security protocols, however require to consider particular equational theories that are not naturally studied in classical automated reasoning. Sometimes, even new concepts have been introduced. One example is the finite variant property [38], which is used in several tools, e.g., *Akiss* [3], Maude-NPA [43] and Tamarin [47]. Another example is the notion of asymmetric unification [42] which is a variant of unification used in Maude-NPA to perform important *syntactic* pruning techniques of the search space, even when reasoning modulo an equational theory. For each of these topics we need to design efficient decision procedures for a variety of equational theories.

3.2.2. Dedicated procedures and tools

We will also design dedicated techniques for automated protocol verification. While existing techniques for security protocol verification are efficient and have reached maturity for verification of confidentiality and authentication properties (or more generally safety properties), our goal is to go beyond these properties and the standard attacker models, verifying the properties and attacker models identified in Section 3.1 . This includes techniques that

- can analyse *indistinguishability* properties, including for instance anonymity and unlinkability properties, but also properties stated in simulation-based (also known as universally composable) frameworks, which express the security of a protocol as an ideal (correct by design) system;
- take into account protocols that rely on *mutable global state* which does not arise in traditional protocols, but is essential when verifying tamper-resistant hardware devices, e.g., the RSA PKCS#11 standard, IBM's CCA and the trusted platform module (TPM);
- consider attacker models for protocols relying on *weak secrets* that need to be copied or remembered by a human, such as multi-factor authentication.

These goals are beyond the scope of most current analysis tools and require both theoretical advances in the area of verification, as well as the design of new efficient verification tools.

3.3. Design

Given our experience in formal analysis of security protocols, including both protocol proofs and findings of flaws, it is tempting to use our experience to design protocols with security in mind and security proofs. This part includes both provably secure design techniques, as well as the development of new protocols.

3.3.1. General design techniques

Design techniques will include *composition results* that allow one to design protocols in a modular way [39], [36]. Composition results come in many flavours: they may allow one to compose protocols with different objectives, e.g. compose a key exchange protocol with a protocol that requires a shared key or rely on a protocol for secure channel establishment, compose different protocols in parallel that may re-use some key material, or compose different sessions of a same protocol.

Another area where composition is of particular importance is Service Oriented Computing, where an "orchestrator" must combine some available component services, while guaranteeing some security properties. In this context, we will work on the automated synthesis of the orchestrator or monitors for enforcing the security goals. These problems require to study new classes of automata that communicate with structured messages.

3.3.2. New protocol design

We will also design new protocols. Application areas that seem of particular importance are:

- External hardware devices such as security APIs that allow one for flexible key management, including key revocation, and their integration in security protocols. The security *fiasco* of the PKCS#11 standard [35], [41] witnesses the need for new protocols in this area.
- Election systems that provide strong security guarantees. We already work (in collaboration with the Caramba team) on a prototype implementation of an e-voting system, Belenios (http://belenios.gforge.inria.fr).
- Mechanisms for publishing personal information (e.g. on social networks) in a controlled way.

PI.R2 Project-Team

3. Research Program

3.1. Proof theory and the Curry-Howard correspondence

3.1.1. Proofs as programs

Proof theory is the branch of logic devoted to the study of the structure of proofs. An essential contributor to this field is Gentzen [57] who developed in 1935 two logical formalisms that are now central to the study of proofs. These are the so-called "natural deduction", a syntax that is particularly well-suited to simulate the intuitive notion of reasoning, and the so-called "sequent calculus", a syntax with deep geometric properties that is particularly well-suited for proof automation.

Proof theory gained a remarkable importance in computer science when it became clear, after genuine observations first by Curry in 1958 [52], then by Howard and de Bruijn at the end of the 60's [70], [89], that proofs had the very same structure as programs: for instance, natural deduction proofs can be identified as typed programs of the ideal programming language known as λ-calculus.

This proofs-as-programs correspondence has been the starting point to a large spectrum of researches and results contributing to deeply connect logic and computer science. In particular, it is from this line of work that Coquand and Huet's Calculus of Constructions [49], [50] stemmed out – a formalism that is both a logic and a programming language and that is at the source of the Coq system [87].

3.1.2. Towards the calculus of constructions

The λ-calculus, defined by Church [48], is a remarkably succinct model of computation that is defined via only three constructions (abstraction of a program with respect to one of its parameters, reference to such a parameter, application of a program to an argument) and one reduction rule (substitution of the formal parameter of a program by its effective argument). The λ-calculus, which is Turing-complete, i.e. which has the same expressiveness as a Turing machine (there is for instance an encoding of numbers as functions in λ-calculus), comes with two possible semantics referred to as call-by-name and call-by-value evaluations. Of these two semantics, the first one, which is the simplest to characterise, has been deeply studied in the last decades [44].

To explain the Curry-Howard correspondence, it is important to distinguish between intuitionistic and classical logic: following Brouwer at the beginning of the 20th century, classical logic is a logic that accepts the use of reasoning by contradiction while intuitionistic logic proscribes it. Then, Howard's observation is that the proofs of the intuitionistic natural deduction formalism exactly coincide with programs in the (simply typed) λ-calculus.

A major achievement has been accomplished by Martin-Löf who designed in 1971 a formalism, referred to as modern type theory, that was both a logical system and a (typed) programming language [80].

In 1985, Coquand and Huet [49], [50] in the Formel team of Inria-Rocquencourt explored an alternative approach based on Girard-Reynolds' system F [58], [83]. This formalism, called the Calculus of Constructions, served as logical foundation of the first implementation of Coq in 1984. Coq was called CoC at this time.

3.1.3. The Calculus of Inductive Constructions

The first public release of CoC dates back to 1989. The same project-team developed the programming language Caml (nowadays called OCaml and coordinated by the Gallium team) that provided the expressive and powerful concept of algebraic data types (a paragon of it being the type of lists). In CoC, it was possible to simulate algebraic data types, but only through a not-so-natural not-so-convenient encoding.

In 1989, Coquand and Paulin [51] designed an extension of the Calculus of Constructions with a generalisation of algebraic types called inductive types, leading to the Calculus of Inductive Constructions (CIC) that started to serve as a new foundation for the Coq system. This new system, which got its current definitive name Coq, was released in 1991.

In practice, the Calculus of Inductive Constructions derives its strength from being both a logic powerful enough to formalise all common mathematics (as set theory is) and an expressive richly-typed functional programming language (like ML but with a richer type system, no effects and no non-terminating functions).

3.2. The development of Coq

Since 1984, about 40 persons have contributed to the development of Coq, out of which 7 persons have contributed to bring the system to the place it is now. First Thierry Coquand through his foundational theoretical ideas, then Gérard Huet who developed the first prototypes with Thierry Coquand and who headed the Coq group until 1998, then Christine Paulin who was the main actor of the system based on the CIC and who headed the development group from 1998 to 2006. On the programming side, important steps were made by Chet Murthy who raised Coq from the prototypical state to a reasonably scalable system, Jean-Christophe Filliâtre who turned to concrete the concept of a small trustful certification kernel on which an arbitrary large system can be set up, Bruno Barras and Hugo Herbelin who, among other extensions, reorganised Coq on a new smoother and more uniform basis able to support a new round of extensions for the next decade.

The development started from the Formel team at Rocquencourt but, after Christine Paulin got a position in Lyon, it spread to École Normale Supérieure de Lyon. Then, the task force there globally moved to the University of Orsay when Christine Paulin got a new position there. On the Rocquencourt side, the part of Formel involved in ML moved to the Cristal team (now Gallium) and Formel got renamed into Coq. Gérard Huet left the team and Christine Paulin started to head a Coq team bilocalised at Rocquencourt and Orsay. Gilles Dowek became the head of the team which was renamed into LogiCal. Following Gilles Dowek who got a position at École Polytechnique, LogiCal moved to the new Inria Saclay research center. It then split again, giving birth to ProVal. At the same time, the Marelle team (formerly Lemme, formerly Croap) which has been a long partner of the Formel team, invested more and more energy in the formalisation of mathematics in Coq, while contributing importantly to the development of Coq, in particular nowadays for what regards user interfaces.

After various other spreadings resulting from where the wind pushed former PhD students, the development of Coq got multi-site with the development now realised by employees of Inria, the CNAM and Paris 7.

We next briefly describe the main components of Coq.

3.2.1. The underlying logic and the verification kernel

The architecture adopts the so-called de Bruijn principle: the well-delimited *kernel* of Coq ensures the correctness of the proofs validated by the system. The kernel is rather stable with modifications tied to the evolution of the underlying Calculus of Inductive Constructions formalism. The kernel includes an interpreter of the programs expressible in the CIC and this interpreter exists in two flavours: a customisable lazy evaluation machine written in OCaml and a call-by-value bytecode interpreter written in C dedicated to efficient computations. The kernel also provides a module system.

3.2.2. Programming and specification languages

The concrete user language of Coq, called *Gallina*, is a high-level language built on top of the CIC. It includes a type inference algorithm, definitions by complex pattern-matching, implicit arguments, mathematical notations and various other high-level language features. This high-level language serves both for the development of programs and for the formalisation of mathematical theories. Coq also provides a large set of commands. Gallina and the commands together forms the *Vernacular* language of Coq.

3.2.3. Standard library

The standard library is written in the vernacular language of Coq. There are libraries for various arithmetical structures and various implementations of numbers (Peano numbers, implementation of $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{Q}$ with binary digits, implementation of $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{Q}$ using machine words, axiomatisation of $\mathbb{R}$). There are libraries for lists, list of a specified length, sorts, and for various implementations of finite maps and finite sets. There are libraries on relations, sets, orders.

3.2.4. Tactics

The tactics are the methods available to conduct proofs. This includes the basic inference rules of the CIC, various advanced higher level inference rules and all the automation tactics. Regarding automation, there are tactics for solving systems of equations, for simplifying ring or field expressions, for arbitrary proof search, for semi-decidability of first-order logic and so on. There is also a powerful and popular untyped scripting language for combining tactics into more complex tactics.

Note that all tactics of Coq produce proof certificates that are checked by the kernel of Coq. As a consequence, possible bugs in proof methods do not hinder the confidence in the correctness of the Coq checker. Note also that the CIC being a programming language, tactics can have their core written (and certified) in the own language of Coq if needed.

3.2.5. Extraction

Extraction is a component of Coq that maps programs (or even computational proofs) of the CIC to functional programs (in OCaml, Scheme or Haskell). Especially, a program certified by Coq can further be extracted to a program of a full-fledged programming language then benefiting of the efficient compilation, linking tools, profiling tools, ... of the target software.

3.3. Dependently typed programming languages

Dependently typed programming (shortly DTP) is an emerging concept referring to the diffuse and broadening tendency to develop programming languages with type systems able to express program properties finer than the usual information of simply belonging to specific data-types. The type systems of dependently-typed programming languages allow to express properties *dependent* of the input and the output of the program (for instance that a sorting program returns a list of same size as its argument). Typical examples of such languages were the Cayenne language, developed in the late 90's at Chalmers University in Sweden and the DML language developed at Boston. Since then, various new tools have been proposed, either as typed programming languages whose types embed equalities (Ωmega at Portland, ATS at Boston, ...) or as hybrid logic/programming frameworks (Agda at Chalmers University, Twelf at Carnegie, Delphin at Yale, OpTT at U. Iowa, Epigram at Nottingham, ...).

DTP contributes to a general movement leading to the fusion between logic and programming. Coq, whose language is both a logic and a programming language which moreover can be extracted to pure ML code plays a role in this movement and some frameworks combining logic and programming have been proposed on top of Coq (Concoqtion at Rice and Colorado, Ynot at Harvard, Why in the ProVal team at Inria). It also connects to Hoare logic, providing frameworks where pre- and post-conditions of programs are tied with the programs.

DTP approached from the programming language side generally benefits of a full-fledged language (e.g. supporting effects) with efficient compilation. DTP approached from the logic side generally benefits of an expressive specification logic and of proof methods so as to certify the specifications. The weakness of the approach from logic however is generally the weak support for effects or partial functions.

3.3.1. Type-checking and proof automation

In between the decidable type systems of conventional data-types based programming languages and the full expressiveness of logically undecidable formulae, an active field of research explores a spectrum of decidable or semi-decidable type systems for possible use in dependently typed programming languages. At the beginning of the spectrum, this includes, for instance, the system F's extension ML_F of the ML type system or the generalisation of abstract data types with type constraints (G.A.D.T.) such as found in the Haskell programming language. At the other side of the spectrum, one finds arbitrary complex type specification languages (e.g. that a sorting function returns a list of type “sorted list”) for which more or less powerful proof automation tools exist – generally first-order ones.

3.4. Around and beyond the Curry-Howard correspondence

For two decades, the Curry-Howard correspondence has been limited to the intuitionistic case but since 1990, an important stimulus spurred on the community following Griffin’s discovery that this correspondence was extensible to classical logic. The community then started to investigate unexplored potential connections between computer science and logic. One of these fields is the computational understanding of Gentzen’s sequent calculus while another one is the computational content of the axiom of choice.

3.4.1. Control operators and classical logic

Indeed, a significant extension of the Curry-Howard correspondence has been obtained at the beginning of the 90’s thanks to the seminal observation by Griffin [59] that some operators known as control operators were typable by the principle of double negation elimination ($\neg\neg A \Rightarrow A$), a principle that enables classical reasoning.

Control operators are used to jump from one location of a program to another. They were first considered in the 60’s by Landin [76] and Reynolds [82] and started to be studied in an abstract way in the 80’s by Felleisen *et al* [55], leading to Parigot’s $\lambda\mu$-calculus [81], a reference calculus that is in close Curry-Howard correspondence with classical natural deduction. In this respect, control operators are fundamental pieces to establish a full connection between proofs and programs.

3.4.2. Sequent calculus

The Curry-Howard interpretation of sequent calculus started to be investigated at the beginning of the 90’s. The main technicality of sequent calculus is the presence of *left introduction* inference rules, for which two kinds of interpretations are applicable. The first approach interprets left introduction rules as construction rules for a language of patterns but it does not really address the problem of the interpretation of the implication connective. The second approach, started in 1994, interprets left introduction rules as evaluation context formation rules. This line of work led in 2000 to the design by Hugo Herbelin and Pierre-Louis Curien of a symmetric calculus exhibiting deep dualities between the notion of programs and evaluation contexts and between the standard notions of call-by-name and call-by-value evaluation semantics.

3.4.3. Abstract machines

Abstract machines came as an intermediate evaluation device, between high-level programming languages and the computer microprocessor. The typical reference for call-by-value evaluation of λ-calculus is Landin’s SECD machine [75] and Krivine’s abstract machine for call-by-name evaluation [72], [71]. A typical abstract machine manipulates a state that consists of a program in some environment of bindings and some evaluation context traditionally encoded into a “stack”.

3.4.4. Delimited control

Delimited control extends the expressiveness of control operators with effects: the fundamental result here is a completeness result by Filinski [56]: any side-effect expressible in monadic style (and this covers references, exceptions, states, dynamic bindings, ...) can be simulated in λ-calculus equipped with delimited control.

3.5. Effective higher-dimensional algebra

3.5.1. Higher-dimensional algebra

Like ordinary categories, higher-dimensional categorical structures originate in algebraic topology. Indeed, ∞-groupoids have been initially considered as a unified point of view for all the information contained in the homotopy groups of a topological space X: the *fundamental ∞-groupoid*$\Pi(X)$ of X contains the elements of X as 0-dimensional cells, continuous paths in X as 1-cells, homotopies between continuous paths as 2-cells, and so on. This point of view translates a topological problem (to determine if two given spaces X and Y are homotopically equivalent) into an algebraic problem (to determine if the fundamental groupoids $\Pi(X)$ and $\Pi(Y)$ are equivalent).

In the last decades, the importance of higher-dimensional categories has grown fast, mainly with the new trend of *categorification* that currently touches algebra and the surrounding fields of mathematics. Categorification is an informal process that consists in the study of higher-dimensional versions of known algebraic objects (such as higher Lie algebras in mathematical physics [43]) and/or of "weakened" versions of those objects, where equations hold only up to suitable equivalences (such as weak actions of monoids and groups in representation theory [54]).

Since a few years, the categorification process has reached logic, with the introduction of homotopy type theory. After a preliminary result that had identified categorical structures in type theory [69], it has been observed recently that the so-called "identity types" are naturally equiped with a structure of ∞-groupoid: the 1-cells are the proofs of equality, the 2-cells are the proofs of equality between proofs of equality, and so on. The striking ressemblance with the fundamental ∞-groupoid of a topological space led to the conjecture that homotopy type theory could serve as a replacement of set theory as a foundational language for different fields of mathematics, and homotopical algebra in particular.

3.5.2. Higher-dimensional rewriting

Higher-dimensional categories are algebraic structures that contain, in essence, computational aspects. This has been recognised by Street [86], and independently by Burroni [47], when they have introduced the concept of *computad* or *polygraph* as combinatorial descriptions of higher categories. Those are directed presentations of higher-dimensional categories, generalising word and term rewriting systems.

In the recent years, the algebraic structure of polygraph has led to a new theory of rewriting, called *higher-dimensional rewriting*, as a unifying point of view for usual rewriting paradigms, namely abstract, word and term rewriting [73], [79], [60], [61], and beyond: Petri nets [63] and formal proofs of classical and linear logic have been expressed in this framework [62]. Higher-dimensional rewriting has developed its own methods to analyse computational properties of polygraphs, using in particular algebraic tools such as derivations to prove termination, which in turn led to new tools for complexity analysis [46].

3.5.3. Squier theory

The homotopical properties of higher categories, as studied in mathematics, are in fact deeply related to the computational properties of their polygraphic presentations. This connection has its roots in a tradition of using rewriting-like methods in algebra, and more specifically in the work of Anick [41] and Squier [85], [84] in the 1980s: Squier has proved that, if a monoid M can be presented by a *finite*, *terminating* and *confluent* rewriting system, then its third integral homology group $H_3(M,\mathbb{Z})$ is finitely generated and the monoid M has *finite derivation type* (a property of homotopical nature). This allowed him to conclude that finite convergent rewriting systems were not a universal solution to decide the word problem of finitely generated monoids. Since then, Yves Guiraud and Philippe Malbos have shown that this connection was part of a deeper unified theory when formulated in the higher-dimensional setting [9], [10], [66], [67], [68].

In particular, the computational content of Squier's proof has led to a constructive methodology to produce, from a convergent presentation, *coherent presentations* and *polygraphic resolutions* of algebraic structures, such as monoids [9] and algebras [65]. A coherent presentation of a monoid M is a 3-dimensional combinatorial object that contains not only a presentation of M (generators and relations), but also higher-dimensional cells, each of which corresponding to two fundamentally different proofs of the same equality: this is, in essence, the same as the proofs of equality of proofs of equality in homotopy type theory. When this process of "unfolding" proofs of equalities is pursued in every dimension, one gets a polygraphic resolution of the starting monoid M. This object has the following desirable qualities: it is free and homotopically equivalent to M (in the canonical model structure of higher categories [74], [42]). A polygraphic resolution of an algebraic object X is a faithful formalisation of X on which one can perform computations, such as homotopical or homological invariants of X. In particular, this has led to new algorithms and proofs in representation theory [7], and in homological algebra [64], [65].

POLSYS Project-Team

3. Research Program

3.1. Introduction

Polynomial system solving is a fundamental problem in Computer Algebra with many applications in cryptography, robotics, biology, error correcting codes, signal theory, ... Among all available methods for solving polynomial systems, computation of Gröbner bases remains one of the most powerful and versatile method since it can be applied in the continuous case (rational coefficients) as well as in the discrete case (finite fields). Gröbner bases are also a building blocks for higher level algorithms who compute real sample points in the solution set of polynomial systems, decide connectivity queries and quantifier elimination over the reals. The major challenge facing the designer or the user of such algorithms is the intrinsic exponential behaviour of the complexity for computing Gröbner bases. The current proposal is an attempt to tackle these issues in a number of different ways: improve the efficiency of the fundamental algorithms (even when the complexity is exponential), develop high performance implementation exploiting parallel computers, and investigate new classes of structured algebraic problems where the complexity drops to polynomial time.

3.2. Fundamental Algorithms and Structured Systems

Participants: Jean-Charles Faugère, Mohab Safey El Din, Elias Tsigaridas, Guénaël Renault, Dongming Wang, Jérémy Berthomieu, Thibaut Verron.

Efficient algorithms F_4/F_5[0] for computing the Gröbner basis of a polynomial system rely heavily on a connection with linear algebra. Indeed, these algorithms reduce the Gröbner basis computation to a sequence of Gaussian eliminations on several submatrices of the so-called Macaulay matrix in some degree. Thus, we expect to improve the existing algorithms by
(i) developing dedicated linear algebra routines performing the Gaussian elimination steps: this is precisely the objective 2 described below;
(ii) generating smaller or simpler matrices to which we will apply Gaussian elimination.
We describe here our goals for the latter problem. First, we focus on algorithms for computing a Gröbner basis of *general polynomial systems*. Next, we present our goals on the development of dedicated algorithms for computing Gröbner bases of *structured polynomial systems* which arise in various applications.

Algorithms for general systems. Several degrees of freedom are available to the designer of a Gröbner basis algorithm to generate the matrices occurring during the computation. For instance, it would be desirable to obtain matrices which would be almost triangular or very sparse. Such a goal can be achieved by considering various interpretations of the F_5 algorithm with respect to different monomial orderings. To address this problem, the tight complexity results obtained for F_5 will be used to help in the design of such a general algorithm. To illustrate this point, consider the important problem of solving boolean polynomial systems; it might be interesting to preserve the sparsity of the original equations and, at the same time, using the fact that overdetermined systems are much easier to solve.

Algorithms dedicated to *structured* polynomial systems. A complementary approach is to exploit the structure of the input polynomials to design specific algorithms. Very often, problems coming from applications are not random but are highly structured. The specific nature of these systems may vary a lot: some polynomial systems can be sparse (when the number of terms in each equation is low), overdetermined (the number of the equations is larger than the number of variables), invariants by the action of some finite groups, multi-linear (each equation is linear w.r.t. to one block of variables) or more generally multihomogeneous. In each case, the ultimate goal is to identify large classes of problems whose theoretical/practical complexity drops and to propose in each case dedicated algorithms.

[0] J.-C. Faugère. *A new efficient algorithm for computing Gröbner bases without reduction to zero (F5).* In Proceedings of ISSAC '02, pages 75-83, New York, NY, USA, 2002. ACM.

3.3. Solving Systems over the Reals and Applications.

Participants: Mohab Safey El Din, Daniel Lazard, Elias Tsigaridas, Ivan Bannwarth.

We shall develop algorithms for solving polynomial systems over complex/real numbers. Again, the goal is to extend significantly the range of reachable applications using algebraic techniques based on Gröbner bases and dedicated linear algebra routines. Targeted application domains are global optimization problems, stability of dynamical systems (e.g. arising in biology or in control theory) and theorem proving in computational geometry.

The following functionalities shall be requested by the end-users:
(i) deciding the emptiness of the real solution set of systems of polynomial equations and inequalities,
(ii) quantifier elimination over the reals or complex numbers,
(iii) answering connectivity queries for such real solution sets.
We will focus on these functionalities.

We will develop algorithms based on the so-called critical point method to tackle systems of equations and inequalities (problem *(i)*) . These techniques are based on solving 0-dimensional polynomial systems encoding "critical points" which are defined by the vanishing of minors of jacobian matrices (with polynomial entries). Since these systems are highly structured, the expected results of Objective 1 and 2 may allow us to obtain dramatic improvements in the computation of Gröbner bases of such polynomial systems. This will be the foundation of practically fast implementations (based on singly exponential algorithms) outperforming the current ones based on the historical Cylindrical Algebraic Decomposition (CAD) algorithm (whose complexity is doubly exponential in the number of variables). We will also develop algorithms and implementations that allow us to analyze, at least locally, the topology of solution sets in some specific situations. A long-term goal is obviously to obtain an analysis of the global topology.

3.4. Low level implementation and Dedicated Algebraic Computation and Linear Algebra.

Participants: Jean-Charles Faugère, Christian Eder, Elias Tsigaridas.

Here, the primary objective is to focus on *dedicated* algorithms and software for the linear algebra steps in Gröbner bases computations and for problems arising in Number Theory. As explained above, linear algebra is a key step in the process of computing efficiently Gröbner bases. It is then natural to develop specific linear algebra algorithms and implementations to further strengthen the existing software. Conversely, Gröbner bases computation is often a key ingredient in higher level algorithms from Algebraic Number Theory. In these cases, the algebraic problems are very particular and specific. Hence dedicated Gröbner bases algorithms and implementations would provide a better efficiency.

Dedicated linear algebra tools.FGB is an efficient library for Gröbner bases computations which can be used, for instance, via MAPLE. However, the library is sequential. A goal of the project is to extend its efficiency to new trend parallel architectures such as clusters of multi-processor systems in order to tackle a broader class of problems for several applications. Consequently, our first aim is to provide a durable, long term software solution, which will be the successor of the existing FGB library. To achieve this goal, we will first develop a high performance linear algebra package (under the LGPL license). This could be organized in the form of a collaborative project between the members of the team. The objective is not to develop a general library similar to the LINBOX project but to propose a dedicated linear algebra package taking into account the specific properties of the matrices generated by the Gröbner bases algorithms. Indeed these matrices are sparse (the actual sparsity depends strongly on the application), almost block triangular and not necessarily of full rank. Moreover, most of the pivots are known at the beginning of the computation. In practice, such matrices are huge (more than 10^6 columns) but taking into account their shape may allow us to speed up the computations by one or several orders of magnitude. A variant of a Gaussian elimination algorithm together with a corresponding C implementation has been presented. The main peculiarity is the order in which the operations are performed. This will be the kernel of the new linear algebra library that will be developed.

Fast linear algebra packages would also benefit to the transformation of a Gröbner basis of a zero–dimensional ideal with respect to a given monomial ordering into a Gröbner basis with respect to another ordering. In the generic case at least, the change of ordering is equivalent to the computation of the minimal polynomial of a so-called multiplication matrix. By taking into account the sparsity of this matrix, the computation of the Gröbner basis can be done more efficiently using a variant of the Wiedemann algorithm. Hence, our goal is also to obtain a dedicated high performance library for transforming (i.e. change ordering) Gröbner bases.

Dedicated algebraic tools for Algebraic Number Theory. Recent results in Algebraic Number Theory tend to show that the computation of Gröbner basis is a key step toward the resolution of difficult problems in this domain [0]. Using existing resolution methods is simply not enough to solve relevant problems. The main algorithmic bottleneck to overcome is to adapt the Gröbner basis computation step to the specific problems. Typically, problems coming from Algebraic Number Theory usually have a lot of symmetries or the input systems are very structured. This is the case in particular for problems coming from the algorithmic theory of Abelian varieties over finite fields [0] where the objects are represented by polynomial system and are endowed with intrinsic group actions. The main goal here is to provide dedicated algebraic resolution algorithms and implementations for solving such problems. We do not restrict our focus on problems in positive characteristic. For instance, tower of algebraic fields can be viewed as triangular sets; more generally, related problems (e.g. effective Galois theory) which can be represented by polynomial systems will receive our attention. This is motivated by the fact that, for example, computing small integer solutions of Diophantine polynomial systems in connection with Coppersmith's method would also gain in efficiency by using a dedicated Gröbner bases computations step.

3.5. Solving Systems in Finite Fields, Applications in Cryptology and Algebraic Number Theory.

Participants: Jean-Charles Faugère, Ludovic Perret, Guénaël Renault, Jérémy Berthomieu.

Here, we focus on solving polynomial systems over finite fields (i.e. the discrete case) and the corresponding applications (Cryptology, Error Correcting Codes, ...). Obviously this objective can be seen as an application of the results of the two previous objectives. However, we would like to emphasize that it is also the source of new theoretical problems and practical challenges. We propose to develop a systematic use of *structured systems* in *algebraic cryptanalysis*.
(i) So far, breaking a cryptosystem using algebraic techniques could be summarized as modeling the problem by algebraic equations and then computing a, usually, time consuming Gröbner basis. A new trend in this field is to require a theoretical complexity analysis. This is needed to explain the behavior of the attack but also to help the designers of new cryptosystems to propose actual secure parameters.
(ii) To assess the security of several cryptosystems in symmetric cryptography (block ciphers, hash functions, ...), a major difficulty is the size of the systems involved for this type of attack. More specifically, the bottleneck is the size of the linear algebra problems generated during a Gröbner basis computation.

We propose to develop a systematic use of *structured systems* in *algebraic cryptanalysis*.

The first objective is to build on the recent breakthrough in attacking McEliece's cryptosystem: it is the first structural weakness observed on one of the oldest public key cryptosystem. We plan to develop a well founded framework for assessing the security of public key cryptosystems based on coding theory from the algebraic cryptanalysis point of view. The answer to this issue is strongly related to the complexity of solving bihomogeneous systems (of bidegree $(1, d)$). We also plan to use the recently gained understanding on the complexity of structured systems in other areas of cryptography. For instance, the MinRank problem – which can be modeled as an overdetermined system of bilinear equations – is at the heart of the structural attack proposed by Kipnis and Shamir against HFE (one of the most well known multivariate public cryptosystem). The same family of structured systems arises in the algebraic cryptanalysis of the Discrete Logarithmic

[0] P. Gaudry, *Index calculus for abelian varieties of small dimension and the elliptic curve discrete logarithm problem*, Journal of Symbolic Computation 44,12 (2009) pp. 1690-1702

[0] e.g. point counting, discrete logarithm, isogeny.

Problem (DLP) over curves (defined over some finite fields). More precisely, some bilinear systems appear in the polynomial modeling the points decomposition problem. Moreover, in this context, a natural group action can also be used during the resolution of the considered polynomial system.

Dedicated tools for linear algebra problems generated during the Gröbner basis computation will be used in algebraic cryptanalysis. The promise of considerable algebraic computing power beyond the capability of any standard computer algebra system will enable us to attack various cryptosystems or at least to propose accurate secure parameters for several important cryptosystems. Dedicated linear tools are thus needed to tackle these problems. From a theoretical perspective, we plan to further improve the theoretical complexity of the hybrid method and to investigate the problem of solving polynomial systems with noise, i.e. some equations of the system are incorrect. The hybrid method is a specific method for solving polynomial systems over finite fields. The idea is to mix exhaustive search and Gröbner basis computation to take advantage of the over-determinacy of the resulting systems.

Polynomial system with noise is currently emerging as a problem of major interest in cryptography. This problem is a key to further develop new applications of algebraic techniques; typically in side-channel and statistical attacks. We also emphasize that recently a connection has been established between several classical lattice problems (such as the Shortest Vector Problem), polynomial system solving and polynomial systems with noise. The main issue is that there is no sound algorithmic and theoretical framework for solving polynomial systems with noise. The development of such framework is a long-term objective.

POSET Team

3. Research Program

3.1. Research Program

Our research programs is structured into three complementary research axis : models, languages and systems, allowing us to develop our multi-disciplinary approach while validating each progress in the related specific fields of computer science ranging among computer music, multi-modal system design, reactive and real-time programing, typed functional programming, formal languages, graph representation theory, applied algebra, logic in computer science, etc.

3.1.1. Models

Inverse semigroup theory has recently been shown [13], [7], [12] [20] to unify most string-based, tree-based or even graph-based modeling approaches. It thus provides a consistent and robust mathematical framework to model the sequential, parallel and reactive aspects of temporal media. Developing the mathematical foundations of our proposal amounts to:

- studying the combinatorial and algorithmic properties of the emerging algebra-based model of structured temporal media,
- developing formal techniques and tools for expressing and verifying properties of temporal media programs especially with a view towards capturing temporal media programing by constraint satisfaction approaches,
- deriving from the known generators of these models adequate sets of application-oriented modeling functions.

3.1.2. Languages

Functional programming is the key link between well-defined mathematical structures and their computerized realizations. Based on functional programming frameworks such as Haskell [0], we are prototyping a Domain Specific Language (DSL) [10] [15] dedicated to the programming of interactive temporal media programming. In this research axis, we aim more specifically at

- designing a robust and modular software architecture that allows to reuse existing pieces of software as well as simply combining them together with new ones,
- defining and implementing a DSL for programming interactive multimedia systems via a simple algebra-based high-level and multi-scale control and combination layer,
- finding the right balance between generic views of temporal media when seen as abstract temporal frames and their specializations when representing concrete gestures, sound, audio, videos, animations, etc.

3.1.3. Systems

Multi-modal interactive systems gather various techniques to capture and analyze gestures, and to combine, transform and produce temporal media. Through regular experiments in collaboration with artists, we also aim at assessing, refining and extending the applicability of our proposal by:

- developing a robust and mathematically well-founded representation of systems and of their behaviors, both programmatic and visual,
- developing and evaluating the adequacy of the GUI induced by this representation when used by artists,
- relating the new models with more classical models of music formalisms and, beyond, other temporal media such as animations, videos, etc.

[0] See [31] for an historical presentation of the Haskell programming language.

PRIVATICS Project-Team (section vide)

PROSECCO Project-Team

3. Research Program

3.1. Symbolic verification of cryptographic applications

Despite decades of experience, designing and implementing cryptographic applications remains dangerously error-prone, even for experts. This is partly because cryptographic security is an inherently hard problem, and partly because automated verification tools require carefully-crafted inputs and are not widely applicable. To take just the example of TLS, a widely-deployed and well-studied cryptographic protocol designed, implemented, and verified by security experts, the lack of a formal proof about all its details has regularly led to the discovery of major attacks (including several in 2014) on both the protocol and its implementations, after many years of unsuspecting use.

As a result, the automated verification for cryptographic applications is an active area of research, with a wide variety of tools being employed for verifying different kinds of applications.

In previous work, the we have developed the following three approaches:

- ProVerif: a symbolic prover for cryptographic protocol models
- Tookan: an attack-finder for PKCS#11 hardware security devices
- F7: a security typechecker for cryptographic applications written in F#

3.1.1. Verifying cryptographic protocols with ProVerif

Given a model of a cryptographic protocol, the problem is to verify that an active attacker, possibly with access to some cryptographic keys but unable to guess other secrets, cannot thwart security goals such as authentication and secrecy [42]; it has motivated a serious research effort on the formal analysis of cryptographic protocols, starting with [40] and eventually leading to effective verification tools, such as our tool ProVerif.

To use ProVerif, one encodes a protocol model in a formal language, called the applied pi-calculus, and ProVerif abstracts it to a set of generalized Horn clauses. This abstraction is a small approximation: it just ignores the number of repetitions of each action, so ProVerif is still very precise, more precise than, say, tree automata-based techniques. The price to pay for this precision is that ProVerif does not always terminate; however, it terminates in most cases in practice, and it always terminates on the interesting class of *tagged protocols* [36]. ProVerif also distinguishes itself from other tools by the variety of cryptographic primitives it can handle, defined by rewrite rules or by some equations, and the variety of security properties it can prove: secrecy [34], [25], correspondences (including authentication) [35], and observational equivalences [33]. Observational equivalence means that an adversary cannot distinguish two processes (protocols); equivalences can be used to formalize a wide range of properties, but they are particularly difficult to prove. Even if the class of equivalences that ProVerif can prove is limited to equivalences between processes that differ only by the terms they contain, these equivalences are useful in practice and ProVerif is the only tool that proves equivalences for an unbounded number of sessions.

Using ProVerif, it is now possible to verify large parts of industrial-strength protocols, such as TLS [30], JFK [26], and Web Services Security [32], against powerful adversaries that can run an unlimited number of protocol sessions, for strong security properties expressed as correspondence queries or equivalence assertions. ProVerif is used by many teams at the international level, and has been used in more than 30 research papers (references available at http://proverif.inria.fr/proverif-users.html).

3.1.2. Verifying security APIs using Tookan

Security application programming interfaces (APIs) are interfaces that provide access to functionality while also enforcing a security policy, so that even if a malicious program makes calls to the interface, certain security properties will continue to hold. They are used, for example, by cryptographic devices such as smartcards and Hardware Security Modules (HSMs) to manage keys and provide access to cryptographic functions whilst keeping the keys secure. Like security protocols, their design is security critical and very difficult to get right. Hence formal techniques have been adapted from security protocols to security APIs.

The most widely used standard for cryptographic APIs is RSA PKCS#11, ubiquitous in devices from smartcards to HSMs. A 2003 paper highlighted possible flaws in PKCS#11 [37], results which were extended by formal analysis work using a Dolev-Yao style model of the standard [38]. However at this point it was not clear to what extent these flaws affected real commercial devices, since the standard is underspecified and can be implemented in many different ways. The Tookan tool, developed by Steel in collaboration with Bortolozzo, Centenaro and Focardi, was designed to address this problem. Tookan can reverse engineer the particular configuration of PKCS#11 used by a device under test by sending a carefully designed series of PKCS#11 commands and observing the return codes. These codes are used to instantiate a Dolev-Yao model of the device's API. This model can then be searched using a security protocol model checking tool to find attacks. If an attack is found, Tookan converts the trace from the model checker into the sequence of PKCS#11 queries needed to make the attack and executes the commands directly on the device. Results obtained by Tookan are remarkable: of 18 commercially available PKCS#11 devices tested, 10 were found to be susceptible to at least one attack.

3.1.3. Verifying cryptographic applications using F7 and F*

Verifying the implementation of a protocol has traditionally been considered much harder than verifying its model. This is mainly because implementations have to consider real-world details of the protocol, such as message formats, that models typically ignore. This leads to a situation that a protocol may have been proved secure in theory, but its implementation may be buggy and insecure. However, with recent advances in both program verification and symbolic protocol verification tools, it has become possible to verify fully functional protocol implementations in the symbolic model.

One approach is to extract a symbolic protocol model from an implementation and then verify the model, say, using ProVerif. This approach has been quite successful, yielding a verified implementation of TLS in F# [30]. However, the generated models are typically quite large and whole-program symbolic verification does not scale very well.

An alternate approach is to develop a verification method directly for implementation code, using well-known program verification techniques such as typechecking. F7 [28] is a refinement typechecker for F#, developed jointly at Microsoft Research Cambridge and Inria. It implements a dependent type-system that allows us to specify security assumptions and goals as first-order logic annotations directly inside the program. It has been used for the modular verification of large web services security protocol implementations [31]. F* (see below) is an extension of F7 with higher-order kinds and a certifying typechecker. Both F7 and F* have a growing user community. The cryptographic protocol implementations verified using F7 and F* already represent the largest verified cryptographic applications to our knowledge.

3.2. Computational verification of cryptographic applications

Proofs done by cryptographers in the computational model are mostly manual. Our goal is to provide computer support to build or verify these proofs. In order to reach this goal, we have already designed the automatic tool CryptoVerif, which generates proofs by sequences of games. Much work is still needed in order to develop this approach, so that it is applicable to more protocols. We also plan to design and implement techniques for proving implementations of protocols secure in the computational model, by generating them from CryptoVerif specifications that have been proved secure, or by automatically extracting CryptoVerif models from implementations.

A different approach is to directly verify cryptographic applications in the computational model by typing. A recent work [41] shows how to use refinement typechecking in F7 to prove computational security for protocol implementations. In this method, henceforth referred to as computational F7, typechecking is used as the main step to justify a classic game-hopping proof of computational security. The correctness of this method is based on a probabilistic semantics of F# programs and crucially relies on uses of type abstraction and parametricity to establish strong security properties, such as indistinguishability.

In principle, the two approaches, typechecking and game-based proofs, are complementary. Understanding how to combine these approaches remains an open and active topic of research.

An alternative to direct computation proofs is to identify the cryptographic assumptions under which symbolic proofs, which are typically easier to derive automatically, can be mapped to computational proofs. This line of research is sometimes called computational soundness and the extent of its applicability to real-world cryptographic protocols is an active area of investigation.

3.3. F*: A Higher-Order Effectful Language Designed for Program Verification

F* [43] is a verification system for ML programs developed collaboratively by Inria and Microsoft Research. ML types are extended with logical predicates that can conveniently express precise specifications for programs (pre- and post- conditions of functions as well as stateful invariants), including functional correctness and security properties. The F* typechecker implements a weakest-precondition calculus to produce first-order logic formulas that are automatically discharged using the Z3 SMT solver. The original F* implementation has been successfully used to verify nearly 50,000 lines of code, including cryptographic protocol implementations, web browser extensions, cloudhosted web applications, and key parts of the F* typechecker and compiler (itself written in F*). F* has also been used for formalizing the semantics of other languages, including JavaScript and a compiler from a subset of F* to JavaScript, and TS*, a secure subset of TypeScript. Programs verified with F* can be extracted to F#, OCaml, C, and JavaScript and then efficiently executed and integrated into larger code bases.

The latest version of F* is written entirely in F*, and bootstraps in OCaml and F#. It is open source and under active development on GitHub. A detailed description of this new F* version is available in a POPL 2016 paper [20] and a POPL 2017 one [6]. We continue to evolve and develop F* and we use it to develop large case studies of verified cryptographic applications, such as miTLS.

3.4. Efficient Formally Secure Compilers to a Tagged Architecture

Severe low-level vulnerabilities abound in today's computer systems, allowing cyber-attackers to remotely gain full control. This happens in big part because our programming languages, compilers, and architectures were designed in an era of scarce hardware resources and too often trade off security for efficiency. The semantics of mainstream low-level languages like C is inherently insecure, and even for safer languages, establishing security with respect to a high-level semantics does not guarantee the absence of low-level attacks. Secure compilation using the coarse-grained protection mechanisms provided by mainstream hardware architectures would be too inefficient for most practical scenarios.

We aim to leverage emerging hardware capabilities for fine-grained protection to build the first, efficient secure compilers for realistic programming languages, both low-level (the C language) and high-level (ML and F*, a dependently-typed variant). These compilers will provide a secure semantics for all programs and will ensure that high-level abstractions cannot be violated even when interacting with untrusted low-level code. To achieve this level of security without sacrificing efficiency, our secure compilers will target a tagged architecture, which associates a metadata tag to each word and efficiently propagates and checks tags according to software-defined rules. We will experimentally evaluate and carefully optimize the efficiency of our secure compilers on realistic workloads and standard benchmark suites. We will use property-based testing and formal verification to provide high confidence that our compilers are indeed secure. Formally, we will construct machine-checked proofs of full abstraction with respect to a secure high-level semantics. This strong property complements compiler correctness and ensures that no machine-code attacker can do more harm to securely compiled components than a component in the secure source language already could.

3.5. Provably secure web applications

Web applications are fast becoming the dominant programming platform for new software, probably because they offer a quick and easy way for developers to deploy and sell their *app*s to a large number of customers. Third-party web-based apps for Facebook, Apple, and Google, already number in the hundreds of thousands and are likely to grow in number. Many of these applications store and manage private user data, such as health information, credit card data, and GPS locations. To protect this data, applications tend to use an ad hoc combination of cryptographic primitives and protocols. Since designing cryptographic applications is easy to get wrong even for experts, we believe this is an opportune moment to develop security libraries and verification techniques to help web application programmers.

As a typical example, consider commercial password managers, such as LastPass, RoboForm, and 1Password. They are implemented as browser-based web applications that, for a monthly fee, offer to store a user's passwords securely on the web and synchronize them across all of the user's computers and smartphones. The passwords are encrypted using a master password (known only to the user) and stored in the cloud. Hence, no-one except the user should ever be able to read her passwords. When the user visits a web page that has a login form, the password manager asks the user to decrypt her password for this website and automatically fills in the login form. Hence, the user no longer has to remember passwords (except her master password) and all her passwords are available on every computer she uses.

Password managers are available as browser extensions for mainstream browsers such as Firefox, Chrome, and Internet Explorer, and as downloadable apps for Android and Apple phones. So, seen as a distributed application, each password manager application consists of a web service (written in PHP or Java), some number of browser extensions (written in JavaScript), and some smartphone apps (written in Java or Objective C). Each of these components uses a different cryptographic library to encrypt and decrypt password data. How do we verify the correctness of all these components?

We propose three approaches. For client-side web applications and browser extensions written in JavaScript, we propose to build a static and dynamic program analysis framework to verify security invariants. To this end, we have developed two security-oriented type systems for JavaScript, Defensive JavaScript [29] [29] and TS* [45], and used them to guarantee security properties for a number of JavaScript applications. For Android smartphone apps and web services written in Java, we propose to develop annotated JML cryptography libraries that can be used with static analysis tools like ESC/Java to verify the security of application code. For clients and web services written in F# for the .NET platform, we propose to use F* to verify their correctness. We also propose to translate verified F* web applications to JavaScript via a verified compiler that preserves the semantics of F* programs in JavaScript.

3.6. Design and Verification of next-generation protocols: identity, blockchains, and messaging

Building on the our work on verifying and re-designing pre-existing protocols like TLS and Web Security in general, with the resources provided by the NEXTLEAP project, we are working on both designing and verifying new protocols in rapidly emerging areas like identity, blockchains, and secure messaging. These are all areas where existing protocols, such as the heavily used OAuth protocol, are in need of considerable re-design in order to maintain privacy and security properties. Other emerging areas, such as blockchains and secure messaging, can have modifications to existing pre-standard proposals or even a complete 'clean slate' design. As shown by Prosecco's work, newer standards, such as IETF OAuth, W3C Web Crypto, and W3C Web Authentication API, can have vulnerabilities fixed before standardization is complete and heavily deployed. We hope that the tools used by Prosecco can shape the design of new protocols even before they are shipped to standards bodies.

SECRET Project-Team

3. Research Program

3.1. Scientific foundations

Our approach relies on a competence whose impact is much wider than cryptology. Our tools come from information theory, discrete mathematics, probabilities, algorithmics, quantum physics... Most of our work mixes fundamental aspects (study of mathematical objects) and practical aspects (cryptanalysis, design of algorithms, implementations). Our research is mainly driven by the belief that discrete mathematics and algorithmics of finite structures form the scientific core of (algorithmic) data protection.

3.2. Symmetric cryptology

Symmetric techniques are widely used because they are the only ones that can achieve some major features such as high-speed or low-cost encryption, fast authentication, and efficient hashing. It is a very active research area which is stimulated by a pressing industrial demand. The process which has led to the new block cipher standard AES in 2001 was the outcome of a decade of research in symmetric cryptography, where new attacks have been proposed, analyzed and then thwarted by some appropriate designs. However, even if its security has not been challenged so far, it clearly appears that the AES cannot serve as a Swiss knife in all environments. In particular an important challenge raised by several new applications is the design of symmetric encryption schemes with some additional properties compared to the AES, either in terms of implementation performance (low-cost hardware implementation, low latency, resistance against side-channel attacks...) or in terms of functionalities (like authenticated encryption). The past decade has then been characterized by a multiplicity of new proposals. This proliferation of symmetric primitives has been amplified by several public competitions (eSTREAM, SHA-3, CAESAR...) which have encouraged innovative constructions and promising but unconventional designs. We are then facing up to a very new situation where implementers need to make informed choices among more than 40 lightweight block ciphers [0] or 57 new authenticated-encryption schemes [0]. Evaluating the security of all these proposals has then become a primordial task which requires the attention of the community.

In this context we believe that the cryptanalysis effort cannot scale up without an in-depth study of the involved algorithms. Indeed most attacks are described as ad-hoc techniques dedicated to a particular cipher. To determine whether they apply to some other primitives, it is then crucial to formalize them in a general setting. Our approach relies on the idea that a unified description of generic attacks (in the sense that they apply to a large class of primitives) is the only methodology for a precise evaluation of the resistance of all these new proposals, and of their security margins. In particular, such a work prevents misleading analyses based on wrong estimations of the complexity or on non-optimized algorithms. It also provides security criteria which enable designers to guarantee that their primitive resists some families of attacks. The main challenge is to provide a generic description which captures most possible optimizations of the attack.

3.3. Code-based cryptography

Public-key cryptography is one of the key tools for providing network security (SSL, e-commerce, e-banking...). The security of nearly all public-key schemes used today relies on the presumed difficulty of two problems, namely factorization of large integers or computing the discrete logarithm over various groups. The hardness of those problems was questioned in 1994 [0] when Shor showed that a quantum computer could solve them efficiently. Though large enough quantum computers that would be able to threaten the

[0] 35 are described on https://www.cryptolux.org/index.php/Lightweight_Block_Ciphers.

[0] see http://competitions.cr.yp.to/caesar-submissions.html

[0] P. Shor, *Algorithms for quantum computation: Discrete logarithms and factoring*, FOCS 1994.

existing cryptosystems do not exist yet, the cryptographic research community has to get ready and has to prepare alternatives. This line of work is usually referred to as *post-quantum cryptography*. This has become a prominent research field. Most notably, an international call for post-quantum primitives [0] has been launched by the NIST very recently, with a submission deadline in November 2017.

The research of the project-team in this field is focused on the design and cryptanalysis of cryptosystems making use of coding theory. Code-based cryptography is one the main techniques for post-quantum cryptography (together with lattice-based, multivariate, or hash-based cryptography).

3.4. Quantum information

The field of quantum information and computation aims at exploiting the laws of quantum physics to manipulate information in radically novel ways. There are two main applications:

(i) quantum computing, that offers the promise of solving some problems that seem to be intractable for classical computers such as for instance factorization or solving the discrete logarithm problem;

(ii) quantum cryptography, which provides new ways to exchange data in a provably secure fashion. For instance it allows key distribution by using an authenticated channel and quantum communication over an unreliable channel with unconditional security, in the sense that its security can be proven rigorously by using only the laws of quantum physics, even with all-powerful adversaries.

Our team deals with quantum coding theoretic issues related to building a large quantum computer and with quantum cryptography. The first part builds upon our expertise in classical coding theory whereas the second axis focuses on obtaining security proofs for quantum protocols or on devising quantum cryptographic protocols (and more generally quantum protocols related to cryptography). A close relationship with partners working in the whole area of quantum information processing in the Parisian region has also been developed through our participation to the Fédération de Recherche “PCQC” (Paris Centre for Quantum Computing).

[0] http://csrc.nist.gov/groups/ST/post-quantum-crypto/

SPADES Project-Team

3. Research Program

3.1. Introduction

The SPADES research program is organized around three main themes, *Components and contracts*, *Real-time multicore programming*, and *Language-based fault tolerance*, that seek to answer the three key questions identified in Section 2.1 . We plan to do so by developing and/or building on programming languages and techniques based on formal methods and formal semantics (hence the use of *"sound programming"* in the project-team title). In particular, we seek to support design where correctness is obtained by construction, relying on proven tools and verified constructs, with programming languages and programming abstractions designed with verification in mind.

3.2. Components and Contracts

Component-based construction has long been advocated as a key approach to the "correct-by-construction" design of complex embedded systems [65]. Witness component-based toolsets such as UC Berkeley's PTOLEMY [53], Verimag's BIP [36], or the modular architecture frameworks used, for instance, in the automotive industry (AUTOSAR) [28]. For building large, complex systems, a key feature of component-based construction is the ability to associate with components a set of *contracts*, which can be understood as rich behavioral types that can be composed and verified to guarantee a component assemblage will meet desired properties. The goal in this theme is to study the formal foundations of the component-based construction of embedded systems, to develop component and contract theories dealing with real-time, reliability and fault-tolerance aspects of components, and to develop proof-assistant-based tools for the computer-aided design and verification of component-based systems.

Formal models for component-based design are an active area of research (see *e.g.*, [29], [30]). However, we are still missing a comprehensive formal model and its associated behavioral theory able to deal *at the same time* with different forms of composition, dynamic component structures, and quantitative constraints (such as timing, fault-tolerance, or energy consumption). Notions of contracts and interface theories have been proposed to support modular and compositional design of correct-by-construction embedded systems (see *e.g.*, [40], [41] and the references therein), but having a comprehensive theory of contracts that deals with all the above aspects is still an open question [71]. In particular, it is not clear how to accomodate different forms of composition, reliability and fault-tolerance aspects, or to deal with evolving component structures in a theory of contracts.

Dealing in the same component theory with heterogeneous forms of composition, different quantitative aspects, and dynamic configurations, requires to consider together the three elements that comprise a component model: behavior, structure and types. *Behavior* refers to behavioral (interaction and execution) models that characterize the behavior of components and component assemblages (*e.g.*, transition systems and their multiple variants – timed, stochastic, etc.). *Structure* refers to the organization of component assemblages or configurations, and the composition operators they involve. *Types* refer to properties or contracts that can be attached to components and component interfaces to facilitate separate development and ensure the correctness of component configurations with respect to certain properties. Taking into account dynamicity requires to establish an explicit link between behavior and structure, as well as to consider higher-order systems, both of which have a direct impact on types.

We plan to develop our component theory by progressing on two fronts: component calculi, and semantical framework. The work on typed component calculi aims to elicit process calculi that capture the main insights of component-based design and programming and that can serve as a bridge towards actual architecture description and programming language developments. The work on the semantical framework should, in the longer term, provide abstract mathematical models for the more operational and linguistic analysis afforded by component calculi. Our work on component theory will find its application in the development of a COQ-based toolchain for the certified design and construction of dependable embedded systems, which constitutes our third main objective for this axis.

3.3. Real-Time Multicore Programming

Programming real-time systems (*i.e.*, systems whose correct behavior depends on meeting timing constraints) requires appropriate languages (as exemplified by the family of synchronous languages [39]), but also the support of efficient scheduling policies, execution time and schedulability analyses to guarantee real-time constraints (*e.g.*, deadlines) while making the most effective use of available (processing, memory, or networking) resources. Schedulability analysis involves analyzing the worst-case behavior of real-time tasks under a given scheduling algorithm and is crucial to guarantee that time constraints are met in any possible execution of the system. Reactive programming and real-time scheduling and schedulability for multiprocessor systems are old subjects, but they are nowhere as mature as their uniprocessor counterparts, and still feature a number of open research questions [35], [48], in particular in relation with mixed criticality systems. The main goal in this theme is to address several of these open questions.

We intend to focus on two issues: multicriteria scheduling on multiprocessors, and schedulability analysis for real-time multiprocessor systems. Beyond real-time aspects, multiprocessor environments, and multicore ones in particular, are subject to several constraints *in conjunction*, typically involving real-time, reliability and energy-efficiency constraints, making the scheduling problem more complex for both the offline and the online cases. Schedulability analysis for multiprocessor systems, in particular for systems with mixed criticality tasks, is still very much an open research area.

Distributed reactive programming is rightly singled out as a major open issue in the recent, but heavily biased (it essentially ignores recent research in synchronous and dataflow programming), survey by Bainomugisha et al. [35]. For our part, we intend to focus on two questions: devising synchronous programming languages for distributed systems and precision-timed architectures, and devising dataflow languages for multiprocessors supporting dynamicity and parametricity while enjoying effective analyses for meeting real-time, resource and energy constraints in conjunction.

3.4. Language-Based Fault Tolerance

Tolerating faults is a clear and present necessity in networked embedded systems. At the hardware level, modern multicore architectures are manufactured using inherently unreliable technologies [43], [58]. The evolution of embedded systems towards increasingly distributed architectures highlighted in the introductory section means that dealing with partial failures, as in Web-based distributed systems, becomes an important issue. While fault-tolerance is an old and much researched topic, several important questions remain open: automation of fault-tolerance provision, composable abstractions for fault-tolerance, fault diagnosis, and fault isolation.

The first question is related to the old question of “system structure for fault-tolerance” as originally discussed by Randell for software fault tolerance [77], and concerns in part our ability to clearly separate fault-tolerance aspects from the design and programming of purely “functional” aspects of an application. The classical arguments in favor of a clear separation of fault-tolerance concerns from application code revolve around reduced code and maintenance complexity [49]. The second question concerns the definition of appropriate abstractions for the modular construction of fault-tolerant embedded systems. The current set of techniques available for building such systems spans a wide range, including exception handling facilities, transaction management schemes, rollback/recovery schemes, and replication protocols. Unfortunately, these different techniques do not necessarily compose well – for instance, combining exception handling and transactions is non trivial, witness the flurry of recent work on the topic, see *e.g.*, [64] and the references therein –, they have no common semantical basis, and they suffer from limited programming language support. The third question concerns the identification of causes for faulty behavior in component-based assemblages. It is directly related to the much researched area of fault diagnosis, fault detection and isolation [66].

We intend to address these questions by leveraging programming language techniques (programming constructs, formal semantics, static analyses, program transformations) with the goal to achieve provable fault-tolerance, *i.e.*, the construction of systems whose fault-tolerance can be formally ensured using verification tools and proof assistants. We aim in this axis to address some of the issues raised by the above open questions by using aspect-oriented programming techniques and program transformations to automate the inclusion of fault-tolerance in systems (software as well as hardware), by exploiting reversible programming models to investigate composable recovery abstractions, and by leveraging causality analyses to study fault-ascription in component-based systems. Compared to the huge literature on fault-tolerance in general, in particular in the systems area (see *e.g.*, [59] for an interesting but not so recent survey), we find by comparison much less work exploiting formal language techniques and tools to achieve or support fault-tolerance. The works reported in [42], [44], [47], [54], [67], [76], [81] provide a representative sample of recent such works.

A common theme in this axis is the use and exploitation of causality information. Causality, *i.e.*, the logical dependence of an effect on a cause, has long been studied in disciplines such as philosophy [72], natural sciences, law [73], and statistics [74], but it has only recently emerged as an important focus of research in computer science. The analysis of logical causality has applications in many areas of computer science. For instance, tracking and analyzing logical causality between events in the execution of a concurrent system is required to ensure reversibility [70], to allow the diagnosis of faults in a complex concurrent system [61], or to enforce accountability [69], that is, designing systems in such a way that it can be determined without ambiguity whether a required safety or security property has been violated, and why. More generally, the goal of fault-tolerance can be understood as being to prevent certain causal chains from occurring by designing systems such that each causal chain either has its premises outside of the fault model (*e.g.*, by introducing redundancy [59]), or is broken (*e.g.*, by limiting fault propagation [78]).

SPECFUN Project-Team

3. Research Program

3.1. Studying special functions by computer algebra

Computer algebra manipulates symbolic representations of exact mathematical objects in a computer, in order to perform computations and operations like simplifying expressions and solving equations for “closed-form expressions”. The manipulations are often fundamentally of algebraic nature, even when the ultimate goal is analytic. The issue of efficiency is a particular one in computer algebra, owing to the extreme swell of the intermediate values during calculations.

Our view on the domain is that research on the algorithmic manipulation of special functions is anchored between two paradigms:

- adopting linear differential equations as the right data structure for special functions,
- designing efficient algorithms in a complexity-driven way.

It aims at four kinds of algorithmic goals:

- algorithms combining functions,
- functional equations solving,
- multi-precision numerical evaluations,
- guessing heuristics.

This interacts with three domains of research:

- computer algebra, meant as the search for quasi-optimal algorithms for exact algebraic objects,
- symbolic analysis/algebraic analysis;
- experimental mathematics (combinatorics, mathematical physics, ...).

This view is made explicit in the present section.

3.1.1. Equations as a data structure

Numerous special functions satisfy linear differential and/or recurrence equations. Under a mild technical condition, the existence of such equations induces a finiteness property that makes the main properties of the functions decidable. We thus speak of *D-finite functions*. For example, 60 % of the chapters in the handbook [21] describe D-finite functions. In addition, the class is closed under a rich set of algebraic operations. This makes linear functional equations just the right data structure to encode and manipulate special functions. The power of this representation was observed in the early 1990s [74], leading to the design of many algorithms in computer algebra. Both on the theoretical and algorithmic sides, the study of D-finite functions shares much with neighbouring mathematical domains: differential algebra, D-module theory, differential Galois theory, as well as their counterparts for recurrence equations.

3.1.2. Algorithms combining functions

Differential/recurrence equations that define special functions can be recombined [74] to define: additions and products of special functions; compositions of special functions; integrals and sums involving special functions. Zeilberger’s fast algorithm for obtaining recurrences satisfied by parametrised binomial sums was developed in the early 1990s already [75]. It is the basis of all modern definite summation and integration algorithms. The theory was made fully rigorous and algorithmic in later works, mostly by a group in RISC (Linz, Austria) and by members of the team [63], [71], [39], [37], [38], [57]. The past ÉPI Algorithms contributed several implementations (*gfun* [66], *Mgfun* [39]).

3.1.3. Solving functional equations

Encoding special functions as defining linear functional equations postpones some of the difficulty of the problems to a delayed solving of equations. But at the same time, solving (for special classes of functions) is a sub-task of many algorithms on special functions, especially so when solving in terms of polynomial or rational functions. A lot of work has been done in this direction in the 1990s; more intensively since the 2000s, solving differential and recurrence equations in terms of special functions has also been investigated.

3.1.4. Multi-precision numerical evaluation

A major conceptual and algorithmic difference exists for numerical calculations between data structures that fit on a machine word and data structures of arbitrary length, that is, *multi-precision* arithmetic. When multi-precision floating-point numbers became available, early works on the evaluation of special functions were just promising that “most” digits in the output were correct, and performed by heuristically increasing precision during intermediate calculations, without intended rigour. The original theory has evolved in a twofold way since the 1990s: by making computable all constants hidden in asymptotic approximations, it became possible to guarantee a *prescribed* absolute precision; by employing state-of-the-art algorithms on polynomials, matrices, etc, it became possible to have evaluation algorithms in a time complexity that is linear in the output size, with a constant that is not more than a few units. On the implementation side, several original works exist, one of which (*NumGfun* [62]) is used in our DDMF.

3.1.5. Guessing heuristics

“Differential approximation”, or “Guessing”, is an operation to get an ODE likely to be satisfied by a given approximate series expansion of an unknown function. This has been used at least since the 1970s and is a key stone in spectacular applications in experimental mathematics [36]. All this is based on subtle algorithms for Hermite–Padé approximants [25]. Moreover, guessing can at times be complemented by proven quantitative results that turn the heuristics into an algorithm [33]. This is a promising algorithmic approach that deserves more attention than it has received so far.

3.1.6. Complexity-driven design of algorithms

The main concern of computer algebra has long been to prove the feasibility of a given problem, that is, to show the existence of an algorithmic solution for it. However, with the advent of faster and faster computers, complexity results have ceased to be of theoretical interest only. Nowadays, a large track of works in computer algebra is interested in developing fast algorithms, with time complexity as close as possible to linear in their output size. After most of the more pervasive objects like integers, polynomials, and matrices have been endowed with fast algorithms for the main operations on them [44], the community, including ourselves, started to turn its attention to differential and recurrence objects in the 2000s. The subject is still not as developed as in the commutative case, and a major challenge remains to understand the combinatorics behind summation and integration. On the methodological side, several paradigms occur repeatedly in fast algorithms: “divide and conquer” to balance calculations, “evaluation and interpolation” to avoid intermediate swell of data, etc. [30].

3.2. Trusted computer-algebra calculations

3.2.1. Encyclopedias

Handbooks collecting mathematical properties aim at serving as reference, therefore trusted, documents. The decision of several authors or maintainers of such knowledge bases to move from paper books [21], [23], [67] to websites and wikis [0] allows for a more collaborative effort in proof reading. Another step toward further confidence is to manage to generate the content of an encyclopedia by computer-algebra programs, as is the case with the Wolfram Functions Site [0] or DDMF [0]. Yet, due to the lingering doubts about computer-algebra systems, some encyclopedias propose both cross-checking by different systems and handwritten companion paper proofs of their content [0]. As of today, there is no encyclopedia certified with formal proofs.

[0] for instance http://dlmf.nist.gov/ for special functions or http://oeis.org/ for integer sequences

[0] http://functions.wolfram.com/

[0] http://ddmf.msr-inria.inria.fr/1.9.1/ddmf

3.2.2. Computer algebra and symbolic logic

Several attempts have been made in order to extend existing computer-algebra systems with symbolic manipulations of logical formulas. Yet, these works are more about extending the expressivity of computer-algebra systems than about improving the standards of correctness and semantics of the systems. Conversely, several projects have addressed the communication of a proof system with a computer-algebra system, resulting in an increased automation available in the proof system, to the price of the uncertainty of the computations performed by this oracle.

3.2.3. Certifying systems for computer algebra

More ambitious projects have tried to design a new computer-algebra system providing an environment where the user could both program efficiently and elaborate formal and machine-checked proofs of correctness, by calling a general-purpose proof assistant like the Coq system. This approach requires a huge manpower and a daunting effort in order to re-implement a complete computer-algebra system, as well as the libraries of formal mathematics required by such formal proofs.

3.2.4. Semantics for computer algebra

The move to machine-checked proofs of the mathematical correctness of the output of computer-algebra implementations demands a prior clarification about the often implicit assumptions on which the presumably correctly implemented algorithms rely. Interestingly, this preliminary work, which could be considered as independent from a formal certification project, is seldom precise or even available in the literature.

3.2.5. Formal proofs for symbolic components of computer-algebra systems

A number of authors have investigated ways to organize the communication of a chosen computer-algebra system with a chosen proof assistant in order to certify specific components of the computer-algebra systems, experimenting various combinations of systems and various formats for mathematical exchanges. Another line of research consists in the implementation and certification of computer-algebra algorithms inside the logic [70], [49], [59] or as a proof-automation strategy. Normalization algorithms are of special interest when they allow to check results possibly obtained by an external computer-algebra oracle [42]. A discussion about the systematic separation of the search for a solution and the checking of the solution is already clearly outlined in [55].

3.2.6. Formal proofs for numerical components of computer-algebra systems

Significant progress has been made in the certification of numerical applications by formal proofs. Libraries formalizing and implementing floating-point arithmetic as well as large numbers and arbitrary-precision arithmetic are available. These libraries are used to certify floating-point programs, implementations of mathematical functions and for applications like hybrid systems.

3.3. Machine-checked proofs of formalized mathematics

To be checked by a machine, a proof needs to be expressed in a constrained, relatively simple formal language. Proof assistants provide facilities to write proofs in such languages. But, as merely writing, even in a formal language, does not constitute a formal proof just per se, proof assistants also provide a proof checker: a small and well-understood piece of software in charge of verifying the correctness of arbitrarily large proofs. The gap between the low-level formal language a machine can check and the sophistication of an average page of mathematics is conspicuous and unavoidable. Proof assistants try to bridge this gap by offering facilities, like notations or automation, to support convenient formalization methodologies. Indeed, many aspects, from the logical foundation to the user interface, play an important role in the feasibility of formalized mathematics inside a proof assistant.

[0] http://129.81.170.14/~vhm/Table.html

3.3.1. Logical foundations and proof assistants

While many logical foundations for mathematics have been proposed, studied, and implemented, type theory is the one that has been more successfully employed to formalize mathematics, to the notable exception of the Mizar system [60], which is based on set theory. In particular, the calculus of construction (CoC) [40] and its extension with inductive types (CIC) [41], have been studied for more than 20 years and been implemented by several independent tools (like Lego, Matita, and Agda). Its reference implementation, Coq [68], has been used for several large-scale formalizations projects (formal certification of a compiler back-end; four-color theorem). Improving the type theory underlying the Coq system remains an active area of research. Other systems based on different type theories do exist and, whilst being more oriented toward software verification, have been also used to verify results of mainstream mathematics (prime-number theorem; Kepler conjecture).

3.3.2. Computations in formal proofs

The most distinguishing feature of CoC is that computation is promoted to the status of rigorous logical argument. Moreover, in its extension CIC, we can recognize the key ingredients of a functional programming language like inductive types, pattern matching, and recursive functions. Indeed, one can program effectively inside tools based on CIC like Coq. This possibility has paved the way to many effective formalization techniques that were essential to the most impressive formalizations made in CIC.

Another milestone in the promotion of the computations-as-proofs feature of Coq has been the integration of compilation techniques in the system to speed up evaluation. Coq can now run realistic programs in the logic, and hence easily incorporates calculations into proofs that demand heavy computational steps.

Because of their different choice for the underlying logic, other proof assistants have to simulate computations outside the formal system, and indeed fewer attempts to formalize mathematical proofs involving heavy calculations have been made in these tools. The only notable exception, which was finished in 2014, the Kepler conjecture, required a significant work to optimize the rewriting engine that simulates evaluation in Isabelle/HOL.

3.3.3. Large-scale computations for proofs inside the Coq system

Programs run and proved correct inside the logic are especially useful for the conception of automated decision procedures. To this end, inductive types are used as an internal language for the description of mathematical objects by their syntax, thus enabling programs to reason and compute by case analysis and recursion on symbolic expressions.

The output of complex and optimized programs external to the proof assistant can also be stamped with a formal proof of correctness when their result is easier to *check* than to *find*. In that case one can benefit from their efficiency without compromising the level of confidence on their output at the price of writing and certify a checker inside the logic. This approach, which has been successfully used in various contexts, is very relevant to the present research project.

3.3.4. Relevant contributions from the Mathematical Component libraries

Representing abstract algebra in a proof assistant has been studied for long. The libraries developed by the MathComp project for the proof of the Odd Order Theorem provide a rather comprehensive hierarchy of structures; however, they originally feature a large number of instances of structures that they need to organize. On the methodological side, this hierarchy is an incarnation of an original work [43] based on various mechanisms, primarily type inference, typically employed in the area of programming languages. A large amount of information that is implicit in handwritten proofs, and that must become explicit at formalization time, can be systematically recovered following this methodology.

Small-scale reflection [46] is another methodology promoted by the MathComp project. Its ultimate goal is to ease formal proofs by systematically dealing with as many bureaucratic steps as possible, by automated computation. For instance, as opposed to the style advocated by Coq's standard library, decidable predicates are systematically represented using computable boolean functions: comparison on integers is expressed as program, and to state that $a \leq b$ one compares the output of this program run on a and b with $true$. In many cases, for example when a and b are values, one can prove or disprove the inequality by pure computation.

The MathComp library was consistently designed after uniform principles of software engineering. These principles range from simple ones, like naming conventions, to more advanced ones, like generic programming, resulting in a robust and reusable collection of formal mathematical components. This large body of formalized mathematics covers a broad panel of algebraic theories, including of course advanced topics of finite group theory, but also linear algebra, commutative algebra, Galois theory, and representation theory. We refer the interested reader to the online documentation of these libraries [69], which represent about 150,000 lines of code and include roughly 4,000 definitions and 13,000 theorems.

Topics not addressed by these libraries and that might be relevant to the present project include real analysis and differential equations. The most advanced work of formalization on these domains is available in the HOL-Light system [51], [52], [53], although some existing developments of interest [28], [61] are also available for Coq. Another aspect of the MathComp libraries that needs improvement, owing to the size of the data we manipulate, is the connection with efficient data structures and implementations, which only starts to be explored.

3.3.5. User interaction with the proof assistant

The user of a proof assistant describes the proof he wants to formalize in the system using a textual language. Depending on the peculiarities of the formal system and the applicative domain, different proof languages have been developed. Some proof assistants promote the use of a declarative language, when the Coq and Matita systems are more oriented toward a procedural style.

The development of the large, consistent body of MathComp libraries has prompted the need to design an alternative and coherent language extension for the Coq proof assistant [48], [47], enforcing the robustness of proof scripts to the numerous changes induced by code refactoring and enhancing the support for the methodology of small-scale reflection.

The development of large libraries is quite a novelty for the Coq system. In particular any long-term development process requires the iteration of many refactoring steps and very little support is provided by most proof assistants, with the notable exception of Mizar [65]. For the Coq system, this is an active area of research.

SUMO Project-Team

3. Research Program

3.1. Analysis and verification of quantitative systems

The overall objective of this axis is to develop the quantitative aspects of formal methods while maintaining the tractability of verification objectives and progressing toward the management of large systems. This covers the development of relevant modeling formalims, to nicely weave time, costs and probabilities with existing models for concurrency. We plan to further study time(d) Petri nets, networks of timed automata (with synchronous or asynchronous communications), stochastic automata, partially observed Markov decision processes, etc. A second objective is to develop verification methods for such quantitative systems. This covers several aspects: quantitative verification questions (compute an optimal scheduling policy), boolean questions on quantitative features (deciding whether some probability is greater than a threshold), robustness issues (will a system have the same behaviors if some parameter is slightly altered), etc. Our goal is to explore the frontier between decidable and undecidable problems, or more pragmatically tractable and untractable problems. Of course, there is a tradeoff between the expressivity and the tractability of a model. Models that incorporate distributed aspects, probabilities, time, etc, are typically untractable. In such a case, abstraction or approximation techniques are a work around that we will explore.

Here are some more detailed topics that we place in our agenda

- analysis of diagnosability and opacity properties for stochastic systems
- verification of time(d) Petri nets
- robustness analysis for timed or/and stochastic systems
- abstraction techniques for quantitative systems

3.2. Control of quantitative systems

The main objective of this research axis is to explore the quantitative and/or distributed extensions of classical control problems. We envision control in its widest meaning of driving a system in order to guarantee or enforce some extra property (i.e. not guaranteed by the system alone), in a partially or totally observed setting. This property can either be logical (e.g. reachability or safety) or quantitative (e.g. reach some performance level). These problems have of course an offline facet (e.g. controller design, existence of a policy/strategy) and an online facet (e.g. algorithm to select some optimal action at runtime).

Our objectives comprise classical controler synthesis for discrete event systems, with extensions to temporal/stochastic/reward settings. They also cover maintaining or maximizing extra properties as diagnosability or opacity, for example in stochastic systems. We also target further analysis of POMDPs (partially observed Markov decision processes), and multi-agent versions of policy synthesis relying on tools from game theory. We aim at adressing some control problems motivated by industrial applications, that raise issues like the optimal control of timed and stochastic discrete event systems, with concerns like robustness to perturbations and multicriteria optimization. Finally, we also plan to work on modular testing, and on runtime enforcement techniques, in order to garantee extra logical and temporal properties to event flows.

3.3. Management of large or distributed systems

The generic terms of “supervision” or “management” of distributed systems cover problems like control, diagnosis, sensor placement, planning, optimization, (state) estimation, parameter identification, testing, etc. This research axis examines how classical settings for such problems can scale up to large or distributed systems. Our work will be driven by considerations like : how to take advantage of modularity, how to design approximate management algorithms, how to design relevant abstractions to make large systems more tractable, how to deal with models of unknown size, how to design mechanisms to obtain relevant models, etc.

As more specific objectives, let us mention:

- Parametric systems. How to verify properties of distributed systems with an unknown number of components.
- Approximate management methods. We will explore the extension of ideas developed for Bayesian inference in large scale stochastic systems (such as turbo-algorithms for example) to the field of modular dynamic systems. When component interactions are sparse, even if exact management methods are unaccessible (for diagnosis, planning, control, etc.), good approximations based on local computations may be accessible.
- Model abstraction. We will explore techniques to design more tractable abstractions of stochastic dynamic systems defined on large sets of variables.
- Self-modeling, which consists in managing large scale systems that are known by their building rules, but which specific managed instance is only discovered at runtime, and on the fly. The model of the managed system is built on-line, following the needs of the management algorithms.
- Distributed control. We will tackle issues related to asynchronous communications between local controllers, and to abstraction techniques allowing to address large systems.
- Test and enforcement. We will tackle coverage issues for the test of large systems, and the test and enforcement of properties for timed models, or for systems handling data.

3.4. Data driven systems

Data-driven systems are systems whose behavior depends both on explicit workflows (scheduling and durations of tasks, calls to possibly distant services,...) and on the data processed by the system (stored data, parameters of a request, results of a request,...). This family of systems covers workflows that convey data (business processes or information systems), transactional systems (web stores), large databases managed with rules (banking systems), collaborative environments (crowds, health systems), etc. These systems are distributed, modular, and open: they integrate components and sub-services distributed over the web and accept requests from clients. Our objective is to provide validation and supervision tools for such systems. To achieve this goal, we have to solve several challenging tasks:

- provide realistic models, and sound automated abstraction techniques, to reason on models that are reasonable abstractions of real systems. These models should be able to encompass modularity, distribution, in a context where workflows and data aspects are tightly connected.
- address design of data driven systems in a declarative way: declarative models are another way to handle data-driven systems. Rather than defining the explicit workflows and their effects on data, rule-based models state how actions are enacted in terms of the shape (pattern matching) or value of the current data. We think that distributed rewriting rules or attributed grammars can provide a practical yet formal framework for maintenance, by providing a solution to update mandatory documentation during the lifetime of an artifact.
- provide tractable solutions for validation of models. Frequent issues are safety questions (can a system reach some bad configuration?), but also liveness (workflows progess), ... These questions should not only remain decidable on our models, but also with efficient computational methods.
- address QoS management in large reconfigurable systems: Data driven distributed systems often have constraints in terms of QoS. This QoS questions adresse performance issues, but also data quality. This calls for an analysis of quantitative features and for reconfiguration techniques to meet desired QoS.

TAMIS Team

3. Research Program

3.1. Axis 1: Vulnerability analysis

This axis proposes different techniques to discover vulnerabilities in systems. The outcomes of this axis are (a) new techniques to discover system vulnerabilities as well as to analyze them, and (b) to understand the importance of the hardware support.

Most existing approaches used at the engineering level rely on testing and fuzzing. Such techniques consist in simulating the system for various input values, and then checking that the result conforms to a given standard. The problem being the large set of inputs to be potentially tested. Existing solutions propose to extract significant sets by mutating a finite set of inputs. Other solutions, especially concolic testing developed at Microsoft, propose to exploit symbolic executions to extract constraints on new values. We build on those existing work, and extend them with recent techniques based on dissimilarity distances and learning. We also account for the execution environment, and study techniques based on the combination of timing attacks with fuzzing techniques to discover and classify classes of behavior of the system under test.

Techniques such as model checking and static analysis have been used for verifying several types of requirements such as safety and reliability. Recently, several works have attempted to adapt model checking to the detection of security issues. It has clearly been identified that this required to work at the level of binary code. Applying formal techniques to such code requires the development of disassembly techniques to obtain a semantically well-defined model. One of the biggest issues faced with formal analysis is the state space explosion problem. This problem is amplified in our context as representations of data (such as stack content) definitively blow up the state space. We propose to use statistical model checking (SMC) of rare events to efficiently identify problematic behaviors.

We also seek to understand vulnerabilities at the architecture and hardware levels. Particularly, we evaluate vulnerabilities of the interfaces and how an adversary could use them to get access to core assets in the system. One particular mechanism to be investigated is the DMA and the so-called Trustzone. An ad-hoc technique to defend against adversarial DMA-access to memory is to keep key material exclusively in registers. This implies co-analyzing machine code and an accurate hardware model.

3.2. Axis 2: Malware analysis

Axis 1 is concerned with vulnerabilities. Such vulnerabilities can be exploited by an attacker in order to introduce malicious behaviors in a system. Another method to identify vulnerabilities is to analyze malware that exploits them. However, modern malware has a wide variety of analysis avoidance techniques. In particular, attackers obfuscate the code leading to a security exploit. For doing so, recent black hat research suggests hiding constants in program choices via polynomials. Such techniques hinder forensic analysis by making detailed analysis labor intensive and time consuming. The objective of research axis 2 is to obtain a full tool chain for malware analysis starting from (a) the observability of the malware via deobfuscation, and (b) the analysis of the resulting binary file. A complementary objective is to understand how hardware attacks can be exploited by malwares.

We first investigate obfuscation techniques. Several solutions exist to mitigate the packer problem. As an example, we try to reverse the packer and remove the environment evaluation in such a way that it performs the same actions and outputs the resulting binary for further analysis. There is a wide range of techniques to obfuscate malware, which includes flattening and virtualization. We will produce a taxonomy of both techniques and tools. We will first give a particular focus to control flow obfuscation via mixed Boolean algebra, which is highly deployed for malware obfuscation. We recently showed that a subset of them can be broken via SAT-solving and synthesis. Then, we will expand our research to other obfuscation techniques.

Once the malware code has been unpacked/deobfuscated, the resulting binary still needs to be fully understood. Advanced malware often contains multiple stages, multiple exploits and may unpack additional features based on its environment. Ensuring that one understands all interesting execution paths of a malware sample is related to enumerating all of the possible execution paths when checking a system for vulnerabilities. The main difference is that in one case we are interested in finding vulnerabilities and in the other in finding exploitative behavior that may mutate. Still, some of the techniques of Axis 1 can be helpful in analyzing malware. The main challenge for axis 2 is thus to adapt the tools and techniques to deal with binary programs as inputs, as well as the logic used to specify malware behavior, including behavior with potentially rare occurrences. Another challenge is to take mutation into account, which we plan to do by exploiting mining algorithms.

Most recent attacks against hardware are based on fault injection which dynamically modifies the semantics of the code. We demonstrated the possibility to obfuscate code using constraint solver in such a way that the code becomes intentionally hostile while hit by a laser beam. This new form of obfuscation opens a new challenge for secure devices where malicious programs can be designed and uploaded that defeat comprehensive static analysis tools or code reviews, due to their multi-semantic nature. We have shown on several products that such an attack cannot be mitigated with the current defenses embedded in Java cards. In this research, we first aim at extending the work on fault injection, then at developing new techniques to analyze such hostile code. This is done by proposing formal models of fault injection, and then reusing results from our work on obfuscation/deobfuscation.

3.3. Axis 3: Building a secure network stack

To evaluate the techniques developed in Axes 1 and 2, we analyze concrete systems developed not only with industry partners, but also within the team. By using our own systems, we can co-evolve best-practices, while externally developed systems provide realistic challenges especially with respect to analyzing obfuscated malware in the hardware or complex vulnerabilities. In this context, Christian Grothoff (ARP Inria) is currently developing a new Internet, which is supposed to be more secure. This introduces interesting challenges both in terms of vulnerability and malware analysis, and hence should be a great opportunity to mix the competences of all the members of the team.

More precisely, this system intends to challenge the idea that network security is an administrative task, where network administrators shield users with passwords, firewalls, intrusion detection systems and policies. Instead, we want to eliminate administrators that have power over user's data, and as such administrators themselves are liabilities, and because a network design that permits administrative intrusion inherently adds vulnerabilities. Instead, the system should ensure secure communication mechanisms without trusted third parties.

Key challenges we work on include (a) improving scalable secure ad-hoc decentralized routing, including key-value lookup, unicast and multicast communication, (b) protecting meta-data in the overlay using advanced decentralized onion routing, (c) a unified public-key infrastructure and identity management solution that is suitable to replace the Web-of-Trust, X.509, DNSSEC and other legacy methods for naming and identifying services, (d) secure synchronous and asynchronous messaging at scale, providing decentralized alternatives to common online social applications and addressing challenges in protocol evolution and compatibility. Finally, we are currently working on GNU Taler, a new secure privacy-preserving payment system where users never have to authenticate. This system in particular can be used as a concrete test case for the methods developed in the team.

To support this research work, we develop a framework named GNUnet. It provides a clear separation into layers, which facilitates testing and verifying the various components. However, we see that often existing formal verification techniques still do not scale to typical subsystems encountered in practice. Our objective is thus to exploit efficient and scalable formal techniques techniques proposed in Axis 1 together with engineering skills in order to guide the validation (message synchronization, data protection, ...) and reach the best compromise. An additional complication is that we need a validation process that not merely covers the software itself, but also all of its dependencies (such as database, cryptographic libraries and networking libraries). For the Taler-specific hardware, we are envisioning an NFC-powered device, which creates new challenges in terms of securing cryptographic computations in a setting where the adversary has control over the power supply. In such a case, the attacker can drive the environment and modify the behavior of the system as we have shown in Axis 2. Providing the control of the environment is a new vector for attackers.

TASC Project-Team

3. Research Program

3.1. Overview

Basic research is guided by the challenges raised before: to classify and enrich the models, to automate reformulation and resolution, to dissociate declarative and procedural knowledge, to come up with theories and tools that can handle problems involving both continuous and discrete variables, to develop modelling tools and to come up with solving tools that scale well. On the one hand, **classification aspects** of this research are integrated within a knowledge base about combinatorial problem solving: the global constraint catalog (see http://sofdem.github.io/gccat/). On the other hand, **solving aspects** are capitalized within the constraint solving system CHOCO. Lastly, within the framework of its activities of valorisation, teaching and of partnership research, the team uses constraint programming for solving various concrete problems. The challenge is, on one side to increase the visibility of the constraints in the others disciplines of computer science, and on the other side to contribute to a broader diffusion of the constraint programming in the industry.

3.2. Fundamental Research Topics

This part presents the research topics investigated by the project:

- Global Constraints Classification, Reformulation and Filtering,
- Convergence between Discrete and Continuous,
- Dynamic, Interactive and over Constrained Problems,
- Solvers.

These research topics are in fact not independent. The work of the team thus frequently relates transverse aspects such as explained global constraints, Benders decomposition and explanations, flexible and dynamic constraints, linear models and relaxations of constraints.

3.2.1. Constraints Classification, Reformulation and Filtering

In this context our research is focused (a) first on identifying recurring combinatorial structures that can be used for modelling a large variety of optimization problems, and (b) exploit these combinatorial structures in order to come up with efficient algorithms in the different fields of optimization technology. The key idea for achieving point (b) is that many filtering algorithms both in the context of Constraint Programming, Mathematical Programming and Local Search can be interpreted as the maintenance of invariants on specific domains (e.g., graph, geometry). The systematic classification of global constraints and of their relaxation brings a synthetic view of the field. It establishes links between the properties of the concepts used to describe constraints and the properties of the constraints themselves. Together with SICS, the team develops and maintains *a catalog of global constraints*, which describes the semantics of more than 431 constraints, and proposes a unified mathematical model for expressing them. This model is based on graphs, automata and logic formulae and allows to derive filtering methods and automatic reformulation for each constraint in a unified way (see http://www.emn.fr/x-info/sdemasse/gccat/index.html). We consider hybrid methods (i.e., methods that involve more than one optimization technology such as constraint programming, mathematical programming or local search), to draw benefit from the respective advantages of the combined approaches. More fundamentally, the study of hybrid methods makes it possible to compare and connect strategies of resolution specific to each approach for then conceiving new strategies. Beside the works on classical, complete resolution techniques, we also investigate local search techniques from a mathematical point of view. These partly random algorithms have been proven very efficient in practice, although we have little theoretical knowledge on their behaviour, which often makes them problem-specific. Our research in that area is focused on a probabilistic model of local search techniques, from which we want to derive quantified information on their behaviour, in order to use this information directly when designing the algorithms and exploit their performances better. We also consider algorithms that maintain local and global consistencies, for more specific models. Having in mind the trade off between genericity and effectiveness, the effort is put on the efficiency of the algorithms with guarantee on the produced levels of filtering. This effort results in adapting existing techniques of resolution such as graph algorithms. For this purpose we identify necessary conditions of feasibility that can be evaluated by efficient incremental algorithms. Genericity is not neglected in these approaches: on the one hand the constraints we focus on are applicable in many contexts (for example, graph partitioning constraints can be used both in logistics and in phylogeny); on the other hand, this work led to study the portability of such constraints and their independence with specific solvers. This research orientation gathers various work such as strong local consistencies, graph partitioning constraints, geometrical constraints, and optimization and soft constraints. Within the perspective to deal with complex industrial problems, we currently develop meta constraints (e.g. *geost*) handling all together the issues of large-scale problems, dynamic constraints, combination of spatial and temporal dimensions, expression of business rules described with first order logic.

3.2.2. Convergence between Discrete and Continuous

Many industrial problems mix continuous and discrete aspects that respectively correspond to physical (e.g., the position, the speed of an object) and logical (e.g., the identifier, the nature of an object) elements. Typical examples of problems are for instance:

- *Geometrical placement problems* where one has to place in space a set of objects subject to various geometrical constraints (i.e., non-overlapping, distance). In this context, even if the positions of the objects are continuous, the structure of optimal configurations has a discrete nature.
- *Trajectory and mission planning problems* where one has to plan and synchronize the moves of several teams in order to achieve some common goal (i.e., fire fighting, coordination of search in the context of rescue missions, surveillance missions of restricted or large areas).
- *Localization problems in mobile robotic* where a robot has to plan alone (only with its own sensors) its trajectory. This kind of problematic occurs in situations where the GPS cannot be used (e.g., under water or Mars exploration) or when it is not precise enough (e.g., indoor surveillance, observation of contaminated sites).

Beside numerical constraints that mix continuous and integer variables we also have global constraints that involve both type of variables. They typically correspond to graph problems (i.e., graph colouring, domination in a graph) where a graph is dynamically constructed with respect to geometrical and-or temporal constraints. In this context, the key challenge is avoiding decomposing the problem in a discrete and continuous parts as it is traditionally the case. As an illustrative example consider *the wireless network deployment problem*. On the one hand, the continuous part consists of finding out where to place a set of antenna subject to various geometrical constraints. On the other hand, by building an interference graph from the positions of the antenna, the discrete part consists of allocating frequencies to antenna in order to avoid interference. In the context of convergence between discrete and continuous variables, our goals are:

- First to identify and compare typical class of techniques that are used in the context of continuous and discrete solvers.
- To see how one can unify and/or generalize these techniques in order to handle in an integrated way continuous and discrete constraints within the same framework.

3.2.3. Dynamic, Interactive and over Constrained Problems

Some industrial applications are defined by a set of constraints which may change over time, for instance due to an interaction with the user. Many other industrial applications are over-constrained, that is, they are defined by set of constraints which are more or less important and cannot be all satisfied at the same time. Generic, dedicated and explanation-based techniques can be used to deal efficiently with such applications. Especially, these applications rely on the notion of *soft constraints* that are allowed to be (partially) violated. The generic concept that captures a wide variety of soft constraints is the violation measure, which is coupled with specific resolution techniques. Lastly, soft constraints allow to combine the expressive power of global constraints with local search frameworks.

3.2.4. Solvers

- *Discrete solver* Our theoretical work is systematically validated by concrete experimentations. We have in particular for that purpose the CHOCO constraint platform. The team develops and maintains CHOCO initially with the assistance of the laboratory e-lab of Bouygues (G. Rochart), the company Amadeus (F. Laburthe), and others researchers such as N. Jussien and H. Cambazard (4C, INP Grenoble). Since 2008 the main developments are done by Charles Prud'homme and Xavier Lorca. The functionalities of CHOCO are gradually extended with the outcomes of our works: design of constraints, analysis and visualization of explanations, etc. The open source CHOCO library is downloaded on average 450 times each month since 2006. CHOCO is developed in line with the research direction of the team, in an open-minded scientific spirit. Contrarily to other solvers where the efficiency often relies on problem-specific algorithms, CHOCO aims at providing the users both with reusable techniques (based on an up-to-date implementation of the global constraint catalogue) and with a variety of tools to ease the use of these techniques (clear separation between model and resolution, event-based solver, management of the over-constrained problems, explanations, etc.).
- *Discrete continuous* We use discrete convexity to describe filtering for families of constraints: We introduce a propagator for pairs of Sum constraints, where the expressions in the sums respect a form of convexity. This propagator is parametric and can be instantiated for various concrete pairs, including Deviation, Spread, and the conjunction of Linear$\leq$ and Among. We show that despite its generality, our propagator is competitive in theory and practice with state-of-the-art propagators.
- *Constraint programming and verification* Constraint Programming has already had several applications to verification problems. It also has many common ideas with Abstract Interpretation, a theory of approximation of the semantics of programs. In both cases, we are interested in a particular set (solutions in CP, program traces in semantics), which is hard or impossible to compute, and this set is replaced by an over-approximation (consistent domains / abstract domains). Previous works (internship of Julie Laniau, PhD of Marie Pelleau, collaboration with the Abstract Interpretation team at the ENS and Antoine Miné in particular) have exhibited some of these links, and identified some situations where the two fields, Abstract Interpretation and Constraint Programming, can complement each other. It is the case in real-time stream processing languages, where Abstract Interpretation techniques may not be precise enough when analyzing loops. With the PhD of Anicet Bart, we are currently working on using CP techniques to find loop invariants for the Faust language, a functional sound processing language.

This work around the design and the development of solvers thus forms the fourth direction of basic research of the project.

TEA Project-Team

3. Research Program

3.1. Previous Works

The challenges of team TEA support the claim that sound Cyber-Physical System design (including embedded, reactive, and concurrent systems altogether) should consider multi-form time models as a central aspect. In this aim, architectural specifications found in software engineering are a natural focal point to start from. Architecture descriptions organize a system model into manageable components, establish clear interfaces between them, collect domain-specific constraints and properties to help correct integration of components during system design. The definition of a formal design methodology to support heterogeneous or multi-form models of time in architecture descriptions demands the elaboration of sound mathematical foundations and the development of formal calculi and methods to instrument them. This constitutes the research program of team TEA.

System design based on the “synchronous paradigm” has focused the attention of many academic and industrial actors on abstracting non-functional implementation details from system design. This elegant design abstraction focuses on the logic of interaction in reactive programs rather than their timed behavior, allowing to secure functional correctness while remaining an intuitive programming model for embedded systems. Yet, it corresponds to embedded technologies of single cores and synchronous buses from the 90s, and may hardly cover the semantic diversity of distribution, parallelism, heterogeneity, of cyber-physical systems found in 21st century Internet-connected, true-time^{TM}-synchronized clouds, of tomorrow’s grids.

By contrast with a synchronous hypothesis yet from the same era, the polychronous MoCC implemented in the data-flow specification language Signal, available in the Eclipse project POP [0] and in the CCSL standard. [0], are inherently capable of describing multi-clock abstractions of GALS systems. The POP and TimeSquare projects provide tooled infrastructures to refine high-level specifications into real-time streaming applications or locally synchronous and globally asynchronous systems, through a series of model analysis, verification, and synthesis services. These tool-supported refinement and transformation techniques can assist the system engineer from the earliest design stages of requirement specification to the latest stages of synthesis, scheduling and deployment. These characteristics make polychrony much closer to the required semantic for compositional, refinement-based, architecture-driven, system design.

While polychrony was a step ahead of the traditional synchronous hypothesis, CCSL is a leap forward from synchrony and polychrony. The essence of CCSL is “multi-form time” toward addressing all of the domain-specific physical, electronic and logical aspects of cyber-physical system design.

3.2. Modeling Times

To make a sense and eventually formalize the semantics of time in system design, we should most certainly rely on algebraic representations of time found in previous works and introduce the paradigm of "time systems" (type systems to represent time) in a way reminiscent to CCSL. Just as a type system abstracts data carried along operations in a program, a time system abstracts the causal interaction of that program module or hardware element with its environment, its pre and post conditions, its assumptions and guarantees, either logical or numerical, discrete or continuous. Some fundamental concepts of the time systems we envision are present in the clock calculi found in data-flow synchronous languages like Signal or Lustre, yet bound to a particular model of concurrency, hence time.

[0] *Polychrony on Polarsys*, https://www.polarsys.org/projects/polarsys.pop

[0] *Clock Constraints in UML/MARTE CCSL*. C. André, F. Mallet. RR-6540. Inria, 2008. http://hal.inria.fr/inria-00280941

In particular, the principle of refinement type systems [0], is to associate information (data-types) inferred from programs and models with properties pertaining, for instance, to the algebraic domain on their value, or any algebraic property related to its computation: effect, memory usage, pre-post condition, value-range, cost, speed, time, temporal logic [0]. Being grounded on type and domain theories, a time system should naturally be equipped with program analysis techniques based on type inference (for data-type inference) or abstract interpretation (for program properties inference) to help establish formal relations between heterogeneous component "types". Just as a time calculus may formally abstract timed concurrent behaviors of system components, timed relations (abstraction and refinement) represent interaction among components.

Scalability and compositionality requires the use of assume-guarantee reasoning to represent them, and to facilitate composition by behavioral sub-typing, in the spirit of the (static) contract-based formalism proposed by Passerone et al. [0]. Verification problems encompassing heterogeneously timed specifications are common and of great variety: checking correctness between abstract and concrete time models relates to desynchronisation (from synchrony to asynchrony) and scheduling analysis (from synchrony to hardware). More generally, they can be perceived from heterogeneous timing viewpoints (e.g. mapping a synchronous-time software on a real-time middle-ware or hardware).

This perspective demands capabilities not only to inject time models one into the other (by abstract interpretation, using refinement calculi), to compare time abstractions one another (using simulation, refinement, bi-simulation, equivalence relations) but also to prove more specific properties (synchronization, determinism, endochrony). All this formalization effort will allow to effectively perform the tooled validation of common cross-domain properties (e.g. cost v.s. power v.s. performance v.s. software mapping) and tackle equally common yet though case studies such as these linking battery capacity, to on-board CPU performance, to static software schedulability, to logical software correctness and plant controllability: the choice of the right sampling period across the system components.

3.3. Modeling Architectures

To address the formalization of such cross-domain case studies, modeling the architecture formally plays an essential role. An architectural model represents components in a distributed system as boxes with well-defined interfaces, connections between ports on component interfaces, and specifies component properties that can be used in analytical reasoning about the model. Several architectural modeling languages for embedded systems have emerged in recent years, including the SAE AADL [0], SysML [0], UML MARTE [0].

In system design, an architectural specification serves several important purposes. First, it breaks down a system model into manageable components to establish clear interfaces between components. In this way, complexity becomes manageable by hiding details that are not relevant at a given level of abstraction. Clear, formally defined, component interfaces allow us to avoid integration problems at the implementation phase. Connections between components, which specify how components affect each other, help propagate the effects of a change in one component to the linked components.

Most importantly, an architectural model is a repository to share knowledge about the system being designed. This knowledge can be represented as requirements, design artifacts, component implementations, held together by a structural backbone. Such a repository enables automatic generation of analytical models for different aspects of the system, such as timing, reliability, security, performance, energy, etc. Since all the models are generated from the same source, the consistency of assumptions w.r.t. guarantees, of abstractions w.r.t. refinements, used for different analyses becomes easier, and can be properly ensured in a design methodology based on formal verification and synthesis methods.

[0] *Abstract Refinement Types*. N. Vazou, P. Rondon, and R. Jhala. European Symposium on Programming. Springer, 2013.

[0] *LTL types FRP*. A. Jeffrey. Programming Languages meets Program Verification.

[0] *A contract-based formalism for the specification of heterogeneous systems*. L. Benvenistu, et al. FDL, 2008

[0] *Architecture Analysis and Design Language*, AS-5506. SAE, 2004. http://standards.sae.org/as5506b

[0] *System modeling Language*. OMG, 2007. http://www.omg.org/spec/SysML

[0] *UML Profile for MARTE*. OMG, 2009. http://www.omg.org/spec/MARTE

Related works in this aim, and closer in spirit to our approach (to focus on modeling time) are domain-specific languages such as Prelude [0] to model the real-time characteristics of embedded software architectures. Conversely, standard architecture description languages could be based on algebraic modeling tools, such as interface theories with the ECDAR tool [0].

In project TEA, it takes form by the normalization of the AADL standard's formal semantics and the proposal of a time specification annex in the form of related standards, such as CCSL, to model concurrency time and physical properties, and PSL, to model timed traces.

3.4. Scheduling Theory

Based on sound formalization of time and CPS architectures, real-time scheduling theory provides tools for predicting the timing behavior of a CPS which consists of many interacting software and hardware components. Expressing parallelism among software components is a crucial aspect of the design process of a CPS. It allows for efficient partition and exploitation of available resources.

The literature about real-time scheduling [0] provides very mature schedulability tests regarding many scheduling strategies, preemptive or non-preemptive scheduling, uniprocessor or multiprocessor scheduling, etc. Scheduling of data-flow graphs has also been extensively studied in the past decades.

A milestone in this prospect is the development of abstract affine scheduling techniques [0]. It consists, first, of approximating task communication patterns (here Safety-Critical Java threads) using cyclo-static data-flow graphs and affine functions. Then, it uses state of the art ILP techniques to find optimal schedules and concretize them as real-time schedules for Safety Critical Java programs [0][0].

Abstract scheduling, or the use of abstraction and refinement techniques in scheduling borrowed to the theory of abstract interpretation [0] is a promising development toward tooled methodologies to orchestrate thousands of heterogeneous hardware/software blocks on modern CPS architectures (just consider modern cars or aircrafts). It is an issue that simply defies the state of the art and known bounds of complexity theory in the field, and consequently requires a particular address.

To develop the underlying theory of this promising research topic, we first need to deepen the theoretical foundation to establish links between scheduling analysis and abstract interpretation. A theory of time systems would offer the ideal framework to pursue this development. It amounts to representing scheduling constraints, inferred from programs, as types or contract properties. It allows to formalize the target time model of the scheduler (the architecture, its middle-ware, its real-time system) and defines the basic concepts to verify assumptions made in one with promises offered by the other: contract verification or, in this case, synthesis.

3.5. Virtual Prototyping

Virtual Prototyping is the technology of developing realistic simulators from models of a system under design; that is, an emulated device that captures most, if not all, of the required properties of the real system, based on its specifications. A virtual prototype should be run and tested like the real device. Ideally, the real application software would be run on the virtual prototyping platform and produce the same results as the real device with the same sequence of outputs and reported performance measurements. This may be true to some extent only. Some trade-offs have often to be made between the accuracy of the virtual prototype, and time to develop accurate models.

[0] *The Prelude language*. LIFL and ONERA, 2012. http://www.lifl.fr/~forget/prelude.html

[0] *PyECDAR, timed games for timed specifications*. Inria, 2013. https://project.inria.fr/pyecdar

[0] *A survey of hard real-time scheduling for multiprocessor systems*. R. I. Davis and A. Burns. *ACM Computing Survey* 43(4), 2011.

[0] *Buffer minimization in EDF scheduling of data-flow graphs*. A. Bouakaz and J.-P. Talpin. LCTES, ACM, 2013.

[0] *ADFG for the synthesis of hard real-time applications*. A. Bouakaz, J.-P. Talpin, J. Vitek. ACSD, IEEE, June 2012.

[0] *Design of SCJ Level 1 Applications Using Affine Abstract Clocks*. A. Bouakaz and J.-P. Talpin. SCOPES, ACM, 2013.

[0] *La vérification de programmes par interprétation abstraite*. P. Cousot. Séminaire au Collège de France, 2008.

In order to speed-up simulation time, the virtual prototype must trade-off with something. Depending upon the application designer's goals, one may be interested in trading some loss of accuracy in exchange for simulation speed, which leads to constructing simulation models that focus on some design aspects and provide abstraction of others. A simulation model can provide an abstraction of the simulated hardware in three directions:

- *Computation abstraction*. A hardware component computes a high level function by carrying out a series of small steps executed by composing logical gates. In a virtual prototyping environment, it is often possible to compute the high level function directly by using the available computing resources on the simulation host machine, thus abstracting the hardware function.
- *Communication abstraction*. Hardware components communicate together using some wiring, and some protocol to transmit the data. Simulation of the communication and the particular protocol may be irrelevant for the purpose of virtual prototyping: communication can be abstracted into higher level data transmission functions.
- *Timing Abstraction*. In a cycle accurate simulator, there are multiple simulation tasks, and each task makes some progress on each clock cycle, but this slows down the simulation. In a virtual prototyping experiment, one may not need such precise timing information: coarser time abstractions can be defined allowing for faster simulation.

The cornerstone of a virtual prototyping platform is the component that simulates the processor(s) of the platform, and its associated peripherals. Such simulation can be *static* or *dynamic*.

A solution usually adopted to handle time in virtual prototyping is to manage hierarchical time scales, use component abstractions where possible to gain performance, use refinement to gain accuracy where needed. Localized time abstraction may not only yield faster simulation, but facilitate also verification and synthesis (e.g. synchronous abstractions of physically distributed systems). Such an approach requires computations and communications to be harmoniously discretized and abstracted from originally heterogeneous viewpoints onto a structuring, articulating, pivot model, for concerted reasoning about time and scheduling of events in a way that ensures global system specification correctness.

In the short term these component models could be based on libraries of predefined models of different levels of abstractions. Such abstractions are common in large programming workbench for hardware modeling, such as SystemC, but less so, because of the engineering required, for virtual prototyping platforms.

The approach of team TEA provides an additional ingredient in the form of rich component interfaces. It therefore dictates to further investigate the combined use of conventional virtual prototyping libraries, defined as executable abstractions of real hardware, with executable component simulators synthesised from rich interface specifications (using, e.g., conventional compiling techniques used for synchronous programs).

TOCCATA Project-Team

3. Research Program

3.1. Introduction

In the former ProVal project, we have been working on the design of methods and tools for deductive verification of programs. One of our original skills was the ability to conduct proofs by using automatic provers and proof assistants at the same time, depending on the difficulty of the program, and specifically the difficulty of each particular verification condition. We thus believe that we are in a good position to propose a bridge between the two families of approaches of deductive verification presented above. Establishing this bridge is one of the goals of the Toccata project: we want to provide methods and tools for deductive program verification that can offer both a high amount of proof automation and a high guarantee of validity. Toward this objective, a new axis of research was proposed: the development of *certified* analysis tools that are themselves formally proved correct.

The reader should be aware that the word “certified” in this scientific programme means “verified by a formal specification and a formal proof that the program meets this specification”. This differs from the standard meaning of “certified” in an industrial context where it means a conformance to some rigorous process and/or norm. We believe this is the right term to use, as it was used for the *Certified Compiler* project [100], the new conference series *Certified Programs and Proofs*, and more generally the important topics of *proof certificates*.

In industrial applications, numerical calculations are very common (e.g. control software in transportation). Typically they involve floating-point numbers. Some of the members of Toccata have an internationally recognized expertise on deductive program verification involving floating-point computations. Our past work includes a new approach for proving behavioral properties of numerical C programs using Frama-C/Jessie [41], various examples of applications of that approach [61], the use of the Gappa solver for proving numerical algorithms [118], an approach to take architectures and compilers into account when dealing with floating-point programs [62], [111]. We also contributed to the Handbook of Floating-Point Arithmetic [110]. A representative case study is the analysis and the proof of both the method error and the rounding error of a numerical analysis program solving the one-dimension acoustic wave equation [4] [54]. Our experience led us to a conclusion that verification of numerical programs can benefit a lot from combining automatic and interactive theorem proving [56], [61]. Certification of numerical programs is the other main axis of Toccata.

Our scientific programme in structured into four objectives:

1. deductive program verification;
2. automated reasoning;
3. formalization and certification of languages, tools and systems;
4. proof of numerical programs.

We detail these objectives below.

3.2. Deductive Program Verification

Permanent researchers: A. Charguéraud, S. Conchon, J.-C. Filliâtre, C. Marché, G. Melquiond, A. Paskevich

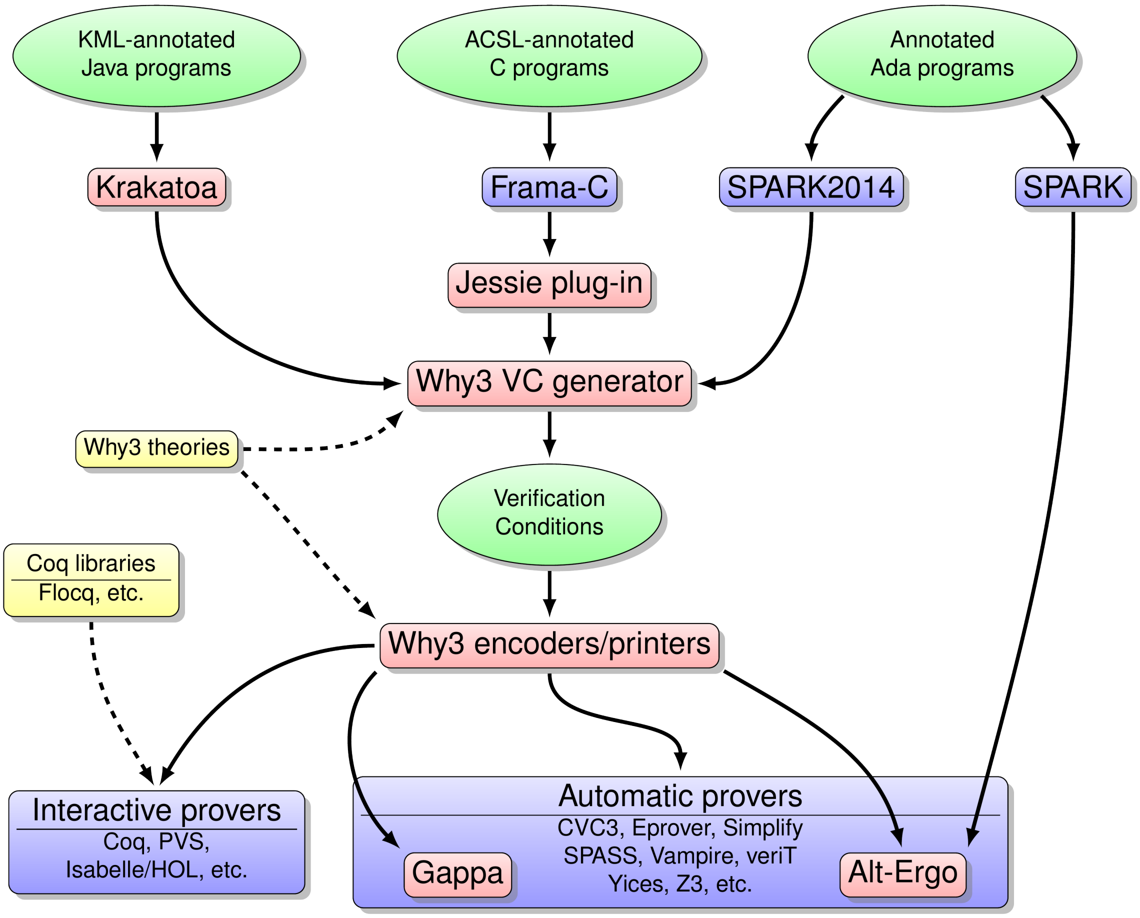


Figure 1. The Why3 ecosystem

3.2.1. The Why3 Ecosystem

This ecosystem is central in our work; it is displayed on Figure 1 . The boxes in red background correspond to the tools we develop in the Toccata team.

- The initial design of Why3 was presented in 2012 [49], [89]. In the past years, the main improvements concern the specification language (such as support for higher-order logic functions [67]) and the support for provers. Several new interactive provers are now supported: PVS 6 (used at NASA), Isabelle2014 (planned to be used in the context of Ada program via Spark), and Mathematica. We also added support for new automated provers: CVC4, Metitarski, Metis, Beagle, Princess, and Yices2. More technical improvements are the design of a Coq tactic to call provers via Why3 from Coq, and the design of a proof session mechanism [48]. Why3 was presented during several invited talks [88], [87], [84], [85].
- At the level of the C front-end of Why3 (via Frama-C), we have proposed an approach to add a notion of refinement on C programs [117], and an approach to reason about pointer programs with a standard logic, via *separation predicates* [47]
- The Ada front-end of Why3 has mainly been developed during the past three years, leading to the release of SPARK2014 [95] (http://www.spark-2014.org/)
- In collaboration with J. Almeida, M. Barbosa, J. Pinto, and B. Vieira (University do Minho, Braga, Portugal), J.-C. Filliâtre has developed a method for certifying programs involving cryptographic methods. It uses Why as an intermediate language [40].
- With M. Pereira and S. Melo de Sousa (Universidade da Beira Interior, Covilhã, Portugal), J.-C. Filliâtre has developed an environment for proving ARM assembly code. It uses Why3 as an intermediate VC generator. It was presented at the Inforum conference [114] (best student paper).

3.2.2. Concurrent Programming

- S. Conchon and A. Mebsout, in collaboration with F. Zaïdi (VALS team, LRI), A. Goel and S. Krstić (Strategic Cad Labs, INTEL) have proposed a new model-checking approach for verifying safety properties of array-based systems. This is a syntactically restricted class of parametrized transition systems with states represented as arrays indexed by an arbitrary number of processes. Cache coherence protocols and mutual exclusion algorithms are typical examples of such systems. It was first presented at CAV 2012 [7] and detailed further [77]. It was applied to the verification of programs with fences [73]. The core algorithm has been extended with a mechanism for inferring invariants. This new algorithm, called BRAB, is able to automatically infer invariants strong enough to prove industrial cache coherence protocols. BRAB computes over-approximations of backward reachable states that are checked to be unreachable in a finite instance of the system. These approximations (candidate invariants) are then model-checked together with the original safety properties. Completeness of the approach is ensured by a mechanism for backtracking on spurious traces introduced by too coarse approximations [74], [106].
- In the context of the ERC DeepSea project [0], A. Charguéraud and his co-authors have developed a unifying semantics for various different paradigms of parallel computing (fork-join, async-finish, and futures), and published a conference paper describing this work [16]. Besides, A. Charguéraud and his co-authors have polished their previous work on granularity control for parallel algorithms using user-provided complexity functions, and produced a journal article [11].

3.2.3. Case Studies

- To provide an easy access to the case studies that we develop using Why3 and its front-ends, we have published a *gallery of verified programs* on our web page http://toccata.lri.fr/gallery/. Part of these examples are the solutions to the competitions VerifyThis 2011 [63], VerifyThis 2012 [3], and the competition VScomp 2011 [90].

[0] Arthur Charguéraud is involved 40% of his time in the ERC DeepSea project, which is hosted at Inria Paris Rocquencourt (team Gallium).

- Other case studies that led to publications are the design of a library of data-structures based on AVLs [66], and the verification a two-lines C program (solving the N-queens puzzle) using Why3 [86].
- A. Charguéraud, with F. Pottier (Inria Paris), extended their formalization of the correctness and asympotic complexity of the classic Union Find data structure, which features the bound expressed in terms of the inverse Ackermann function [39]. The proof, conducted using CFML extended with time credits, was refined using a slightly more complex potential function, allowing to derive a simpler and richer interface for the data structure. A journal article is in preparation.

For other case studies, see also sections of numerical programs and formalization of languages and tools.

3.2.4. Project-team Positioning

Several research groups in the world develop their own approaches, techniques, and tools for deductive verification. With respect to all these related approaches and tools, our originality is our will to use more sophisticated specification languages (with inductive definitions, higher-order features and such) and the ability to use a large set of various theorem provers, including the use of interactive theorem proving to deal with complex functional properties.

- The RiSE team [0] at Microsoft Research Redmond, USA, partly in collaboration with team "programming methodology" team [0] at ETH Zurich develop tools that are closely related to ours: Boogie and Dafny are direct competitors of Why3, VCC is a direct competitor of Frama-C/Jessie.
- The KeY project [0] (several teams, mainly at Karlsruhe and Darmstadt, Germany, and Göteborg, Sweden) develops the KeY tool for Java program verification [38], based on dynamic logic, and has several industrial users. They use a specific modal logic (dynamic logic) for modeling programs, whereas we use standard logic, so as to be able to use off-the-shelf automated provers.
- The "software engineering" group at Augsburg, Germany, develops the KIV system [0], which was created more than 20 years ago (1992) and is still well maintained and efficient. It provides a semi-interactive proof environment based on algebraic-style specifications, and is able to deal with several kinds of imperative style programs. They have a significant industrial impact.
- The VeriFast system [0] aims at verifying C programs specified in Separation Logic. It is developed at the Katholic University at Leuven, Belgium. We do not usually use separation logic (so as to use off-the-shelf provers) but alternative approaches (e.g. static memory separation analysis).
- The Mobius Program Verification Environment [0] is a joint effort for the verification of Java source annotated with JML, combining static analysis and runtime checking. The tool ESC/Java2 [0] is a VC generator similar to Krakatoa, that builds on top of Boogie. It is developed by a community leaded by University of Copenhagen, Denmark. Again, our specificity with respect to them is the consideration of more complex specification languages and interactive theorem proving.
- The Lab for Automated Reasoning and Analysis [0] at EPFL, develop methods and tools for verification of Java (Jahob) and Scala (Leon) programs. They share with us the will and the ability to use several provers at the same time.
- The TLA environment [0], developed by Microsoft Research and the Inria team Veridis, aims at the verification of concurrent programs using mathematical specifications, model checking, and interactive or automated theorem proving.
- The F* project [0], developed by Microsoft Research and the Inria Prosecco team, aims at providing a rich environment for developing programs and proving them.

[0] http://research.microsoft.com/en-us/groups/rise/default.aspx
[0] http://www.pm.inf.ethz.ch/
[0] http://www.key-project.org/
[0] http://www.isse.uni-augsburg.de/en/software/kiv/
[0] http://people.cs.kuleuven.be/~bart.jacobs/verifast/
[0] http://kindsoftware.com/products/opensource/Mobius/
[0] http://kindsoftware.com/products/opensource/ESCJava2/
[0] http://lara.epfl.ch/w/
[0] http://research.microsoft.com/en-us/um/people/lamport/tla/tla.html
[0] http://research.microsoft.com/en-us/projects/fstar/

The KeY and KIV environments mentioned above are partly based on interactive theorem provers. There are other approaches on top of general-purpose proof assistants for proving programs that are not purely functional:

- The Ynot project [0] is a Coq library for writing imperative programs specified in separation logic. It was developed at Harvard University, until the end of the project in 2010. Ynot had similar goals as CFML, although Ynot requires programs to be written in monadic style inside Coq, whereas CFML applies directly on programs written in OCaml syntax, translating them into logical formulae.
- Front-ends to Isabelle were developed to deal with simple sequential imperative programs [116] or C programs [113]. The L4-verified project [96] is built on top of Isabelle.

3.3. Automated Reasoning

Permanent researchers: S. Conchon, G. Melquiond, A. Paskevich

3.3.1. Generalities on Automated Reasoning

- J. C. Blanchette and A. Paskevich have designed an extension to the TPTP TFF (Typed First-order Form) format of theorem proving problems to support rank-1 polymorphic types (also known as ML-style parametric polymorphism) [1]. This extension, named TFF1, has been incorporated in the TPTP standard.
- S. Conchon defended his *habilitation à diriger des recherches* in December 2012. The memoir [70] provides a useful survey of the scientific work of the past 10 years, around the SMT solving techniques, that led to the tools Alt-Ergo and Cubicle as they are nowadays.

3.3.2. Quantifiers and Triggers

- C. Dross, J. Kanig, S. Conchon, and A. Paskevich have proposed a generic framework for adding a decision procedure for a theory or a combination of theories to an SMT prover. This mechanism is based on the notion of instantiation patterns, or *triggers*, which restrict instantiation of universal premises and can effectively prevent a combinatorial explosion. A user provides an axiomatization with triggers, along with a proof of completeness and termination in the proposed framework, and obtains in return a sound, complete and terminating solver for his theory. A prototype implementation was realized on top of Alt-Ergo. As a case study, a feature-rich axiomatization of doubly-linked lists was proved complete and terminating [82]. C. Dross defended her PhD thesis in April 2014 [83]. The main results of the thesis are: (1) a formal semantics of the notion of *triggers* typically used to control quantifier instantiation in SMT solvers, (2) a general setting to show how a first-order axiomatization with triggers can be proved correct, complete, and terminating, and (3) an extended DPLL(T) algorithm to integrate a first-order axiomatization with triggers as a decision procedure for the theory it defines. Significant case studies were conducted on examples coming from SPARK programs, and on the benchmarks on B set theory constructed within the BWare project.

3.3.3. Reasoning Modulo Theories

- S. Conchon, É. Contejean and M. Iguernelala have presented a modular extension of ground AC-completion for deciding formulas in the combination of the theory of equality with user-defined AC symbols, uninterpreted symbols and an arbitrary signature-disjoint Shostak theory X [72]. This work extends the results presented in [71] by showing that a simple preprocessing step allows to get rid of a full AC-compatible reduction ordering, and to simply use a partial multiset extension of a *non-necessarily AC-compatible* ordering.
- S. Conchon, M. Iguernelala, and A. Mebsout have designed a collaborative framework for reasoning modulo simple properties of non-linear arithmetic [76]. This framework has been implemented in the Alt-Ergo SMT solver.

[0] http://ynot.cs.harvard.edu/

- S. Conchon, G. Melquiond and C. Roux have described a dedicated procedure for a theory of floating-point numbers which allows reasoning on approximation errors. This procedure is based on the approach of the Gappa tool: it performs saturation of consequences of the axioms, in order to refine bounds on expressions. In addition to the original approach, bounds are further refined by a constraint solver for linear arithmetic [78]. This procedure has been implemented in Alt-Ergo.
- In collaboration with A. Mahboubi (Inria project-team Typical), and G. Melquiond, the group involved in the development of Alt-Ergo have implemented and proved the correctness of a novel decision procedure for quantifier-free linear integer arithmetic [2]. This algorithm tries to bridge the gap between projection and branching/cutting methods: it interleaves an exhaustive search for a model with bounds inference. These bounds are computed provided an oracle capable of finding constant positive linear combinations of affine forms. An efficient oracle based on the Simplex procedure has been designed. This algorithm is proved sound, complete, and terminating and is implemented in Alt-Ergo.
- Most of the results above are detailed in M. Iguernelala's PhD thesis [93].

3.3.4. Applications

- We have been quite successful in the application of Alt-Ergo to industrial development: qualification by Airbus France, integration of Alt-Ergo into the Spark Pro toolset.
- In the context of the BWare project, aiming at using Why3 and Alt-Ergo for discharging proof obligations generated by Atelier B, we made progress into several directions. The method of translation of B proof obligations into Why3 goals was first presented at ABZ'2012 [109]. Then, new drivers have been designed for Why3, in order to use new back-end provers Zenon modulo and iProver modulo. A notion of rewrite rule was introduced into Why3, and a transformation for simplifying goals before sending them to back-end provers was designed. Intermediate results obtained so far in the project were presented both at the French conference AFADL [81] and at ABZ'2014 [80].

  On the side of Alt-Ergo, recent developments have been made to efficiently discharge proof obligations generated by Atelier B. This includes a new plugin architecture to facilitate experiments with different SAT engines, new heuristics to handle quantified formulas, and important modifications in its internal data structures to boost performances of core decision procedures. Benchmarks realized on more than 10,000 proof obligations generated from industrial B projects show significant improvements [75].
- Hybrid automatons interleave continuous behaviors (described by differential equations) with discrete transitions. D. Ishii and G. Melquiond have worked on an automated procedure for verifying safety properties (that is, global invariants) of such systems [94].

3.3.5. Project-team Positioning

Automated Theorem Proving is a large community, but several sub-groups can be identified:

- The SMT-LIB community gathers people interested in reasoning modulo theories. In this community, only a minority of participants are interested in supporting first-order quantifiers at the same time as theories. SMT solvers that support quantifiers are Z3 (Microsoft Research Redmond, USA), CVC3 and its successor CVC4 [0].
- The TPTP community gathers people interested in first-order theorem proving.
- Other Inria teams develop provers: veriT by team Veridis, and Psyche by team Parsifal.
- Other groups develop provers dedicated to very specific cases, such as Metitarski [0] at Cambridge, UK, which aims at proving formulas on real numbers, in particular involving special functions such as log or exp. The goal is somewhat similar to our CoqInterval library, *cf* objective 4.

[0] http://cvc4.cs.nyu.edu/web/

[0] http://www.cl.cam.ac.uk/~lp15/papers/Arith/

It should be noticed that a large number of provers mentioned above are connected to Why3 as back-ends.

3.4. Formalization and Certification of Languages, Tools and Systems

Permanent researchers: S. Boldo, A. Charguéraud, C. Marché, G. Melquiond, C. Paulin

3.4.1. Real Numbers, Real Analysis, Probabilities

- S. Boldo, C. Lelay, and G. Melquiond have worked on the Coquelicot library, designed to be a user-friendly Coq library about real analysis [59], [60]. An easier way of writing formulas and theorem statements is achieved by relying on total functions in place of dependent types for limits, derivatives, integrals, power series, and so on. To help with the proof process, the library comes with a comprehensive set of theorems and some automation. We have exercised the library on several use cases: on an exam at university entry level [98], for the definitions and properties of Bessel functions [97], and for the solution of the one-dimensional wave equation [99]. We have also conducted a survey on the formalization of real arithmetic and real analysis in various proof systems [12].
- Watermarking techniques are used to help identify copies of publicly released information. They consist in applying a slight and secret modification to the data before its release, in a way that should remain recognizable even in (reasonably) modified copies of the data. Using the Coq ALEA library, which formalizes probability theory and probabilistic programs, D. Baelde together with P. Courtieu, D. Gross-Amblard from Rennes and C. Paulin have established new results about the robustness of watermarking schemes against arbitrary attackers [42]. The technique for proving robustness is adapted from methods commonly used for cryptographic protocols and our work illustrates the strengths and particularities of the ALEA style of reasoning about probabilistic programs.

3.4.2. Formalization of Languages, Semantics

- P. Herms, together with C. Marché and B. Monate (CEA List), has developed a certified VC generator, using Coq. The program for VC calculus and its specifications are both written in Coq, but the code is crafted so that it can be extracted automatically into a stand-alone executable. It is also designed in a way that allows the use of arbitrary first-order theorem provers to discharge the generated obligations [92]. On top of this generic VC generator, P. Herms developed a certified VC generator for C source code annotated using ACSL. This work is the main result of his PhD thesis [91].
- A. Tafat and C. Marché have developed a certified VC generator using Why3 [102], [103]. The challenge was to formalize the operational semantics of an imperative language, and a corresponding weakest precondition calculus, without the possibility to use Coq advanced features such as dependent types or higher-order functions. The classical issues with local bindings, names and substitutions were solved by identifying appropriate lemmas. It was shown that Why3 can offer a significantly higher amount of proof automation compared to Coq.
- A. Charguéraud, together with Alan Schmitt (Inria Rennes) and Thomas Wood (Imperial College), has developed an interactive debugger for JavaScript. The interface, accessible as a webpage in a browser, allows to execute a given JavaScript program, following step by step the formal specification of JavaScript developped in prior work on *JsCert* [50]. Concretely, the tool acts as a double-debugger: one can visualize both the state of the interpreted program and the state of the interpreter program. This tool is intended for the JavaScript committee, VM developpers, and other experts in JavaScript semantics.
- M. Clochard, C. Marché, and A. Paskevich have developed a general setting for developing programs involving binders, using Why3. This approach was successfully validated on two case studies: a verified implementation of untyped lambda-calculus and a verified tableaux-based theorem prover [69].

- M. Clochard, J.-C. Filliâtre, C. Marché, and A. Paskevich have developed a case study on the formalization of semantics of programming languages using Why3 [67]. This case study aims at illustrating recent improvements of Why3 regarding the support for higher-order logic features in the input logic of Why3, and how these are encoded into first-order logic, so that goals can be discharged by automated provers. This case study also illustrates how reasoning by induction can be done without need for interactive proofs, via the use of *lemma functions*.
- M. Clochard and L. Gondelman have developed a formalization of a simple compiler in Why3 [68]. It compiles a simple imperative language into assembler instructions for a stack machine. This case study was inspired by a similar example developed using Coq and interactive theorem proving. The aim is to improve significantly the degree of automation in the proofs. This is achieved by the formalization of a Hoare logic and a Weakest Precondition Calculus on assembly programs, so that the correctness of compilation is seen as a formal specification of the assembly instructions generated.

3.4.3. Project-team Positioning

The objective of formalizing languages and algorithms is very general, and it is pursued by several Inria teams. One common trait is the use of the Coq proof assistant for this purpose: Pi.r2 (development of Coq itself and its meta-theory), Gallium (semantics and compilers of programming languages), Marelle (formalization of mathematics), SpecFun (real arithmetic), Celtique (formalization of static analyzers).

Other environments for the formalization of languages include

- ACL2 system [0]: an environment for writing programs with formal specifications in first-order logic based on a Lisp engine. The proofs are conducted using a prover based on the Boyer-Moore approach. It is a rather old system but still actively maintained and powerful, developed at University of Texas at Austin. It has a strong industrial impact.
- Isabelle environment [0]: both a proof assistant and an environment for developing pure applicative programs. It is developed jointly at University of Cambridge, UK, Technische Universität München, Germany, and to some extent by the VALS team at LRI, Université Paris-Sud. It features highly automated tactics based on ATP systems (the Sledgehammer tool).
- The team “Trustworthy Systems” at NICTA in Australia [0] aims at developing highly trustable software applications. They developed a formally verified micro-kernel called seL4 [96], using a home-made layer to deal with C programs on top of the Isabelle prover.
- The PVS system [0] is an environment for both programming and proving (purely applicative) programs. It is developed at the Computer Science Laboratory of SRI international, California, USA. A major user of PVS is the team LFM [0] at NASA Langley, USA, for the certification of programs related to air traffic control.

In the Toccata team, we do not see these alternative environments as competitors, even though, for historical reasons, we are mainly using Coq. Indeed both Isabelle and PVS are available as back-ends of Why3.

3.5. Proof of Numerical Programs

Permanent researchers: S. Boldo, C. Marché, G. Melquiond

- Linked with objective 1 (Deductive Program Verification), the methodology for proving numerical C programs has been presented by S. Boldo in her habilitation [52] and as invited speaker [53]. An application is the formal verification of a numerical analysis program. S. Boldo, J.-C. Filliâtre, and G. Melquiond, with F. Clément and P. Weis (POMDAPI team, Inria Paris - Rocquencourt), and M. Mayero (LIPN), completed the formal proof of the second-order centered finite-difference scheme for the one-dimensional acoustic wave [55][4].

[0] http://www.cs.utexas.edu/~moore/acl2/

[0] http://isabelle.in.tum.de/

[0] http://ssrg.nicta.com.au/projects/TS/

[0] http://pvs.csl.sri.com/

[0] http://shemesh.larc.nasa.gov/fm/fm-main-team.html

- Several challenging floating-point algorithms have been studied and proved. This includes an algorithm by Kahan for computing the area of a triangle: S. Boldo proved an improvement of its error bound and new investigations in case of underflow [51]. This includes investigations about quaternions. They should be of norm 1, but due to the round-off errors, a drift of this norm is observed over time. C. Marché determined a bound on this drift and formally proved it correct [9]. P. Roux formally verified an algorithm for checking that a matrix is semi-definite positive [115]. The challenge here is that testing semi-definiteness involves algebraic number computations, yet it needs to be implemented using only approximate floating-point operations.
- Because of compiler optimizations (or bugs), the floating-point semantics of a program might change once compiled, thus invalidating any property proved on the source code. We have investigated two ways to circumvent this issue, depending on whether the compiler is a black box. When it is, T. Nguyen has proposed to analyze the assembly code it generates and to verify it is correct [112]. On the contrary, S. Boldo and G. Melquiond (in collaboration with J.-H. Jourdan and X. Leroy) have added support for floating-point arithmetic to the CompCert compiler and formally proved that none of the transformations the compiler applies modify the floating-point semantics of the program [58], [57].
- Linked with objectives 2 (Automated Reasoning) and 3 (Formalization and Certification of Languages, Tools and Systems), G. Melquiond has implemented an efficient Coq library for floating-point arithmetic and proved its correctness in terms of operations on real numbers [107]. It serves as a basis for an interval arithmetic on which Taylor models have been formalized. É. Martin-Dorel and G. Melquiond have integrated these models into CoqInterval [15]. This Coq library is dedicated to automatically proving the approximation properties that occur when formally verifying the implementation of mathematical libraries (libm).
- Double rounding occurs when the target precision of a floating-point computation is narrower than the working precision. In some situations, this phenomenon incurs a loss of accuracy. P. Roux has formally studied when it is innocuous for basic arithmetic operations [115]. É. Martin-Dorel and G. Melquiond (in collaboration with J.-M. Muller) have formally studied how it impacts algorithms used for error-free transformations [105]. These works were based on the Flocq formalization of floating-point arithmetic for Coq.
- By combining multi-precision arithmetic, interval arithmetic, and massively-parallel computations, G. Melquiond (in collaboration with G. Nowak and P. Zimmermann) has computed enough digits of the Masser-Gramain constant to invalidate a 30-year old conjecture about its closed form [108].

3.5.1. Project-team Positioning

This objective deals both with formal verification and floating-point arithmetic, which is quite uncommon. Therefore our competitors/peers are few. We may only cite the works by J. Duracz and M. Konečný, Aston University in Birmingham, UK.

The Inria team AriC (Grenoble - Rhône-Alpes) is closer to our research interests, but they are lacking manpower on the formal proof side; we have numerous collaborations with them. The Inria team Caramel (Nancy - Grand Est) also shares some research interests with us, though fewer; again, they do not work on the formal aspect of the verification; we have some occasional collaborations with them.

There are many formalization efforts from chip manufacturers, such as AMD (using the ACL2 proof assistant) and Intel (using the Forte proof assistants) but the algorithms they consider are quite different from the ones we study. The works on the topic of floating-point arithmetic from J. Harrison at Intel using HOL Light are really close to our research interests, but they seem to be discontinued.

A few deductive program verification teams are willing to extend their tools toward floating-point programs. This includes the KeY project and SPARK. We have an ongoing collaboration with the latter, in the context of the ProofInUSe project.

Deductive verification is not the only way to prove programs. Abstract interpretation is widely used, and several teams are interested in floating-point arithmetic. This includes the Inria team Antique (Paris - Rocquencourt) and a CEA List team, who have respectively developed the Astrée and Fluctuat tools. This approach targets a different class of numerical algorithms than the ones we are interested in.

Other people, especially from the SMT community (*cf* objective 2), are also interested in automatically proving formulas about floating-point numbers, notably at Oxford University. They are mainly focusing on pure floating-point arithmetic though and do not consider them as approximation of real numbers.

Finally, it can be noted that numerous teams are working on the verification of numerical programs, but assuming the computations are real rather than floating-point ones. This is out of the scope of this objective.

VEGAS Project-Team (section vide)

VERIDIS Project-Team

3. Research Program

3.1. Automated and Interactive Theorem Proving

The VeriDis team gathers experts in techniques and tools for automatic deduction and interactive theorem proving, and specialists in methods and formalisms designed for the development of trustworthy concurrent and distributed systems and algorithms. Our common objective is twofold: first, we wish to advance the state of the art in automated and interactive theorem proving, and their combinations. Second, we work on making the resulting technology available for the computer-aided verification of distributed systems and protocols. In particular, our techniques and tools are intended to support sound methods for the development of trustworthy distributed systems that scale to algorithms relevant for practical applications.

VeriDis members from Saarbrücken are developing SPASS [10], one of the leading automated theorem provers for first-order logic based on the superposition calculus [39]. The group also studies general frameworks for the combination of theories such as the locality principle [52] and automated reasoning mechanisms these induce.

In a complementary approach to automated deduction, VeriDis members from Nancy work on techniques for integrating reasoners for specific theories. They develop veriT [1], an SMT (Satisfiability Modulo Theories [41]) solver that combines decision procedures for different fragments of first-order logic and that integrates an automatic theorem prover for full first-order logic. The veriT solver is designed to produce detailed proofs; this makes it particularly suitable as a component of a robust cooperation of deduction tools.

Finally, VeriDis members design effective quantifier elimination methods and decision procedures for algebraic theories, supported by their efficient implementation in the Redlog system [4].

An important objective of this line of work is the integration of theories in automated deduction. Typical theories of interest, including fragments of arithmetic, are not expressible in first-order logic. We therefore explore efficient, modular techniques for integrating semantic and syntactic reasoning methods, develop novel combination results and techniques for quantifier instantiation. These problems are addressed from both sides, e.g. by embedding a decision procedure into the superposition framework or by allowing an SMT solver to accept axiomatizations for plug-in theories. We also develop specific decision procedures for theories such as non-linear real arithmetic that are important when reasoning about certain classes of (e.g., real-time) systems but that also have interesting applications beyond verification.

We rely on interactive theorem provers for reasoning about specifications at a high level of abstraction when fully automatic verification is not (yet) feasible. An interactive proof platform should help verification engineers lay out the proof structure at a sufficiently high level of abstraction; powerful automatic plug-ins should then discharge the resulting proof steps. Members of VeriDis have ample experience in the specification and subsequent machine-assisted, interactive verification of algorithms. In particular, we participate in a project at the joint Microsoft Research-Inria Centre in Saclay on the development of methods and tools for the formal proof of TLA$^+$ [45] specifications. Our prover relies on a declarative proof language, and calls upon several automatic backends [3]. Trust in the correctness of the overall proof can be ensured when the backends provide justifications that can be checked by the trusted kernel of a proof assistant. During the development of a proof, most obligations that are passed to the prover actually fail – for example, because necessary information is not present in the context or because the invariant is too weak, and we are interested in explaining failed proof attempts to the user, in particular through the construction of counter-models.

3.2. Formal Methods for Developing and Analyzing Algorithms and Systems

Theorem provers are not used in isolation, but they support the application of sound methodologies for modeling and verifying systems. In this respect, members of VeriDis have gained expertise and recognition in making contributions to formal methods for concurrent and distributed algorithms and systems [2], [9], and in applying them to concrete use cases. In particular, the concept of *refinement* [38], [40], [48] in state-based modeling formalisms is central to our approach because it allows us to present a rational (re)construction of system development. An important goal in designing such methods is to establish precise proof obligations many of which can be discharged by automatic tools. This requires taking into account specific characteristics of certain classes of systems and tailoring the model to concrete computational models. Our research in this area is supported by carrying out case studies for academic and industrial developments. This activity benefits from and influences the development of our proof tools.

In this line of work, we investigate specific development and verification patterns for particular classes of algorithms, in order to reduce the work associated with their verification. We are also interested in applications of formal methods and their associated tools to the development of systems that underlie specific certification requirements in the sense of, e.g., Common Criteria. Finally, we are interested in the adaptation of model checking techniques for verifying actual distributed programs, rather than high-level models.

Today, the formal verification of a new algorithm is typically the subject of a PhD thesis, if it is addressed at all. This situation is not sustainable given the move towards more and more parallelism in mainstream systems: algorithm developers and system designers must be able to productively use verification tools for validating their algorithms and implementations. On a high level, the goal of VeriDis is to make formal verification standard practice for the development of distributed algorithms and systems, just as symbolic model checking has become commonplace in the development of embedded systems and as security analysis for cryptographic protocols is becoming standard practice today. Although the fundamental problems in distributed programming are well-known, they pose new challenges in the context of modern system paradigms, including ad-hoc and overlay networks or peer-to-peer systems, and they must be integrated for concrete applications.

ACUMES Project-Team

3. Research Program

3.1. Research directions

The project develops along the following two axes:

- modeling complex systems through novel (unconventional) PDE systems, accounting for multi-scale phenomena and uncertainty;
- optimization and optimal control algorithms for systems governed by the above PDE systems.

These themes are motivated by the specific problems treated in the applications, and represent important and up-to-date issues in engineering sciences. For example, improving the design of transportation means and civil buildings, and the control of traffic flows, would result not only in better performances of the object of the optimization strategy (vehicles, buildings or road networks level of service), but also in enhanced safety and lower energy consumption, contributing to reduce costs and pollutant emissions.

3.1.1. PDE models accounting for multi-scale phenomena and uncertainties

Dynamical models consisting of evolutionary PDEs, mainly of hyperbolic type, appear classically in the applications studied by the previous Project-Team Opale (compressible flows, traffic, cell-dynamics, medicine, etc). Yet, the classical purely macroscopic approach is not able to account for some particular phenomena related to specific interactions occurring at smaller scales. These phenomena can be of greater importance when dealing with particular applications, where the "first order" approximation given by the purely macroscopic approach reveals to be inadequate. We refer for example to self-organizing phenomena observed in pedestrian flows [95], or to the dynamics of turbulent flows for which large scale / small scale vortical structures interfere [123].

Nevertheless, macroscopic models offer well known advantages, namely a sound analytical framework, fast numerical schemes, the presence of a low number of parameters to be calibrated, and efficient optimization procedures. Therefore, we are convinced of the interest of keeping this point of view as dominant, while completing the models with information on the dynamics at the small scale / microscopic level. This can be achieved through several techniques, like hybrid models, homogenization, mean field games. In this project, we will focus on the aspects detailed below.

The development of adapted and efficient numerical schemes is a mandatory completion, and sometimes ingredient, of all the approaches listed below. The numerical schemes developed by the team are based on finite volumes or finite elements techniques, and constitute an important tool in the study of the considered models, providing a necessary step towards the design and implementation of the corresponding optimization algorithms, see Section 3.1.2 .

3.1.1.1. Micro-macro couplings

Modeling of complex problems with a dominant macroscopic point of view often requires couplings with small scale descriptions. Accounting for systems heterogeneity or different degrees of accuracy usually leads to coupled PDE-ODE systems.

In the case of heterogeneous problems the coupling is "intrinsic", i.e. the two models evolve together and mutually affect each-other. For example, accounting for the impact of a large and slow vehicle (like a bus or a truck) on traffic flow leads to a strongly coupled system consisting of a (system of) conservation law(s) coupled with an ODE describing the bus trajectory, which acts as a moving bottleneck.The coupling is realized through a local unilateral moving constraint on the flow at the bus location, see [64] for an existence result and [49], [63] for numerical schemes.

If the coupling is intended to offer higher degree of accuracy at some locations, a macroscopic and a microscopic model are connected through an artificial boundary, and exchange information across it through suitable boundary conditions. See [55], [84] for some applications in traffic flow modelling, and [74], [79], [81] for applications to cell dynamics.

The corresponding numerical schemes are usually based on classical finite volume or finite element methods for the PDE, and Euler or Runge-Kutta schemes for the ODE, coupled in order to take into account the interaction fronts. In particular, the dynamics of the coupling boundaries require an accurate handling capturing the possible presence of non-classical shocks and preventing diffusion, which could produce wrong solutions, see for example [49], [63].

We plan to pursue our activity in this framework, also extending the above mentioned approaches to problems in two or higher space dimensions, to cover applications to crowd dynamics or fluid-structure interaction.

3.1.1.2. Micro-macro limits

Rigorous derivation of macroscopic models from microscopic ones offers a sound basis for the proposed modeling approach, and can provide alternative numerical schemes, see for example [56], [66] for the derivation of Lighthill-Whitham-Richards [107], [122] traffic flow model from Follow-the-Leader and [75] for results on crowd motion models (see also [97]). To tackle this aspect, we will rely mainly on two (interconnected) concepts: measure-valued solutions and mean-field limits.

The notion of **measure-valued solutions** for conservation laws was first introduced by DiPerna [67], and extensively used since then to prove convergence of approximate solutions and deduce existence results, see for example [76] and references therein. Measure-valued functions have been recently advocated as the appropriate notion of solution to tackle problems for which analytical results (such as existence and uniqueness of weak solutions in distributional sense) and numerical convergence are missing [38], [78]. We refer, for example, to the notion of solution for non-hyperbolic systems [86], for which no general theoretical result is available at present, and to the convergence of finite volume schemes for systems of hyperbolic conservation laws in several space dimensions, see [78].

In this framework, we plan to investigate and make use of measure-based PDE models for vehicular and pedestrian traffic flows. Indeed, a modeling approach based on (multi-scale) time-evolving measures (expressing the agents probability distribution in space) has been recently introduced (see the monograph [60]), and proved to be successful for studying emerging self-organised flow patterns [59]. The theoretical measure framework proves to be also relevant in addressing micro-macro limiting procedures of mean field type [87], where one lets the number of agents going to infinity, while keeping the total mass constant. In this case, one must prove that the *empirical measure*, corresponding to the sum of Dirac measures concentrated at the agents positions, converges to a measure-valued solution of the corresponding macroscopic evolution equation. We recall that a key ingredient in this approach is the use of the *Wasserstein distances* [130], [131]. Indeed, as observed in [114], the usual L^1 spaces are not natural in this context, since they don't guarantee uniqueness of solutions.

This procedure can potentially be extended to more complex configurations, like for example road networks or different classes of interacting agents, or to other application domains, like cell-dynamics.

Another powerful tool we shall consider to deal with micro-macro limits is the so-called **Mean Field Games (MFG)** technique (see the seminal paper [106]). This approach has been recently applied to some of the systems studied by the team, such as traffic flow and cell dynamics. In the context of crowd dynamics, including the case of several populations with different targets, the mean field game approach has been adopted in [45], [46], [68], [105], under the assumption that the individual behavior evolves according to a stochastic process, which gives rise to parabolic equations greatly simplifying the analysis of the system. Besides, a deterministic context is studied in [118], which considers a non-local velocity field. For cell dynamics, in order to take into account the fast processes that occur in the migration-related machinery, a framework such the one developed in [62] to handle games "where agents evolve their strategies according to the best-reply scheme on a much faster time scale than their social configuration variables" may turn out to be suitable. An alternative framework to MFG is also considered. This framework is based on the formulation of -Nash- games constrained by the **Fokker-Planck** (FP, [36]) partial differential equations that govern the time evolution of the probability density functions -PDF- of stochastic systems and on objectives that may require to follow a given PDF trajectory or to minimize an expectation functional.

3.1.1.3. Non-local flows

Non-local interactions can be described through macroscopic models based on integro-differential equations. Systems of the type

$$\partial_t u + \mathrm{div}_{\mathbf{x}} F(t, \mathbf{x}, u, W) = 0, \qquad t > 0,\ \mathbf{x} \in \mathbb{R}^d,\ d \geq 1, \tag{1}$$

where $u = u(t, \mathbf{x}) \in \mathbb{R}^N$, $N \geq 1$ is the vector of conserved quantities and the variable $W = W(t, x, u)$ depends on an integral evaluation of u, arise in a variety of physical applications. Space-integral terms are considered for example in models for granular flows [33], sedimentation [40], supply chains [89], conveyor belts [90], biological applications like structured populations dynamics [113], or more general problems like gradient constrained equations [34]. Also, non-local in time terms arise in conservation laws with memory, starting from [61]. In particular, equations with non-local flux have been recently introduced in traffic flow modeling to account for the reaction of drivers or pedestrians to the surrounding density of other individuals, see [3], [6] [48], [52], [126]. While pedestrians are likely to react to the presence of people all around them, drivers will mainly adapt their velocity to the downstream traffic, assigning a greater importance to closer vehicles. In particular, and in contrast to classical (without integral terms) macroscopic equations, these models are able to display finite acceleration of vehicles through Lipschitz bounds on the mean velocity [3], [6] and lane formation in crossing pedestrian flows.

General analytical results on non-local conservation laws, proving existence and eventually uniqueness of solutions of the Cauchy problem for (1), can be found in [35] for scalar equations in one space dimension ($N = d = 1$), in [53] for scalar equations in several space dimensions ($N = 1$, $d \geq 1$) and in [29], [54], [58] for multi-dimensional systems of conservation laws. Besides, specific finite volume numerical methods have been developed recently in [29], [6] and [104].

Relying on these encouraging results, we aim to push a step further the analytical and numerical study of non-local models of type (1), in particular concerning well-posedness of initial - regularity of solutions, boundary value problems and high-order numerical schemes.

3.1.1.4. Uncertainty in parameters and initial-boundary data

Different sources of uncertainty can be identified in PDE models, related to the fact that the problem of interest is not perfectly known. At first, initial and boundary condition values can be uncertain. For instance, in traffic flows, the time-dependent value of inlet and outlet fluxes, as well as the initial distribution of vehicles density, are not perfectly determined [47]. In aerodynamics, inflow conditions like velocity modulus and direction, are subject to fluctuations [93], [112]. For some engineering problems, the geometry of the boundary can also be uncertain, due to structural deformation, mechanical wear or disregard of some details [70]. Another source of uncertainty is related to the value of some parameters in the PDE models. This is typically the case of parameters in turbulence models in fluid mechanics, which have been calibrated according to some reference flows but are not universal [124], [129], or in traffic flow models, which may depend on the type of road, weather conditions, or even the country of interest (due to differences in driving rules and conductors behaviour). This leads to equations with flux functions depending on random parameters [125], [128], for which the mean and the variance of the solutions can be computed using different techniques. Indeed, uncertainty quantification for systems governed by PDEs has become a very active research topic in the last years. Most approaches are embedded in a probabilistic framework and aim at quantifying statistical moments of the PDE solutions, under the assumption that the characteristics of uncertain parameters are known. Note that classical Monte-Carlo approaches exhibit low convergence rate and consequently accurate simulations require huge computational times. In this respect, some enhanced algorithms have been proposed, for example in the balance law framework [111]. Different approaches propose to modify the PDE solvers to account for this probabilistic context, for instance by defining the non-deterministic part of the solution on an orthogonal basis (Polynomial Chaos decomposition) and using a Galerkin projection [93], [102], [108], [133] or an entropy closure method [65], or by discretizing the probability space and extending the numerical schemes to the stochastic components [28]. Alternatively, some other approaches maintain a fully deterministic PDE resolution, but approximate the solution in the vicinity of the reference parameter values by Taylor series expansions based on first- or second-order sensitivities [119], [129], [132].

Our objective regarding this topic is twofold. In a pure modeling perspective, we aim at including uncertainty quantification in models calibration and validation for predictive use. In this case, the choice of the techniques will depend on the specific problem considered [39]. Besides, we plan to extend previous works on sensitivity analysis [70], [109] to more complex and more demanding problems. In particular, high-order Taylor expansions of the solution (greater than two) will be considered in the framework of the Sensitivity Equation Method [41] (SEM) for unsteady aerodynamic applications, to improve the accuracy of mean and variance estimations. A second targeted topic in this context is the study of the uncertainty related to turbulence closure parameters, in the sequel of [129]. We aim at exploring the capability of the SEM approach to detect a change of flow topology, in case of detached flows. Our ambition is to contribute to the emergence of a new generation of simulation tools, which will provide solution densities rather than values, to tackle real-life uncertain problems. This task will also include a reflection about numerical schemes used to solve PDE systems, in the perspective of constructing a unified numerical framework able to account for exact geometries (isogeometric methods), uncertainty propagation and sensitivity analysis w.r.t. control parameters.

3.1.2. Optimization and control algorithms for systems governed by PDEs

The non-classical models described above are developed in the perspective of design improvement for real-life applications. Therefore, control and optimization algorithms are also developed in conjunction with these models. The focus here is on the methodological development and analysis of optimization algorithms for PDE systems in general, keeping in mind the application domains in the way the problems are mathematically formulated.

3.1.2.1. Sensitivity VS adjoint equation

Adjoint methods (achieved at continuous or discrete level) are now commonly used in industry for steady PDE problems. Our recent developments [121] have shown that the (discrete) adjoint method can be efficiently applied to cost gradient computations for time-evolving traffic flow on networks, thanks to the special structure of the associated linear systems and the underlying one dimensionality of the problem. However, this strategy is questionable for more complex (e.g. 2D/3D) unsteady problems, because it requires sophisticated and time-consuming check-pointing and/or re-computing strategies [37], [88] for the backward time integration of the adjoint variables. The sensitivity equation method (SEM) offers a promising alternative [69], [98], if the number of design parameters is moderate. Moreover, this approach can be employed for other goals, like fast evaluation of neighboring solutions or uncertainty propagation [70].
Regarding this topic, we intend to apply the continuous sensitivity equation method to challenging problems. In particular, in aerodynamics, multi-scale turbulence models like Large-Eddy Simulation (LES) [123] , Detached-Eddy Simulation (DES) [127] or Organized-Eddy Simulation (OES) [43], are more and more employed to analyse the unsteady dynamics of the flows around bluff-bodies, because they have the ability to compute the interactions of vortices at different scales, contrary to classical Reynolds-Averaged Navier-Stokes models. However, their use in design optimization is tedious, due to the long time integration required. In collaboration with turbulence specialists (M. Braza, CNRS - IMFT), we aim at developing numerical methods for effective sensitivity analysis in this context, and apply them to realistic problems, like the optimization of active flow control devices. Note that the use of SEM allows computing cost functional gradients at any time, which permits to construct new gradient-based optimization strategies like instantaneous-feedback method [100] or multiobjective optimization algorithm (see section below).

3.1.2.2. Multi-objective descent algorithms for multi-disciplinary, multi-point, unsteady optimization or robust-design

n differentiable optimization, multi-disciplinary, multi-point, unsteady optimization or robust-design can all be formulated as multi-objective optimization problems. In this area, we have proposed the *Multiple-Gradient*

Descent Algorithm (MGDA) to handle all criteria concurrently [71] [72]. Originally, we have stated a principle according which, given a family of local gradients, a descent direction common to all considered objective-functions simultaneously is identified, assuming the Pareto-stationarity condition is not satisfied. When the family is linearly-independent, we dispose of a direct algorithm. Inversely, when the family is linearly-dependent, a quadratic-programming problem should be solved. Hence, the technical difficulty is mostly conditioned by the number m of objective functions relative to the search space dimension n. In this respect, the basic algorithm has recently been revised [73] to handle the case where $m > n$, and even $m \gg n$, and is currently being tested on a test-case of robust design subject to a periodic time-dependent Navier-Stokes flow.

The multi-point situation is very similar and, being of great importance for engineering applications, will be treated at large.

Moreover, we intend to develop and test a new methodology for robust design that will include uncertainty effects. More precisely, we propose to employ MGDA to achieve an effective improvement of all criteria simultaneously, which can be of statistical nature or discrete functional values evaluated in confidence intervals of parameters. Some recent results obtained at ONERA [116] by a stochastic variant of our methodology confirm the viability of the approach. A PhD thesis has also been launched at ONERA/DADS.

Lastly, we note that in situations where gradients are difficult to evaluate, the method can be assisted by a meta-model [135].

3.1.2.3. Bayesian Optimization algorithms for efficient computation of general equilibria

Bayesian Optimization -BO- relies on Gaussian processes, which are used as emulators (or surrogates) of the black-box model outputs based on a small set of model evaluations. Posterior distributions provided by the Gaussian process are used to design acquisition functions that guide sequential search strategies that balance between exploration and exploitation. Such approaches have been transposed to frameworks other than optimization, such as uncertainty quantification. Our aim is to investigate how the BO apparatus can be applied to the search of general game equilibria, and in particular the classical Nash equilibrium (NE). To this end, we propose two complementary acquisition functions, one based on a greedy search approach and one based on the Stepwise Uncertainty Reduction paradigm [80]. Our proposal is designed to tackle derivative-free, expensive models, hence requiring very few model evaluations to converge to the solution.

3.1.2.4. Decentralized strategies for inverse problems

Most if not all the mathematical formulations of inverse problems (a.k.a. reconstruction, identification, data recovery, non destructive engineering,...) are known to be ill posed in the Hadamard sense. Indeed, in general, inverse problems try to fulfill (minimize) two or more very antagonistic criteria. One classical example is the Tikhonov regularization, trying to find artificially smoothed solutions close to naturally non-smooth data.

We consider here the theoretical general framework of parameter identification coupled to (missing) data recovery. Our aim is to design, study and implement algorithms derived within a game theoretic framework, which are able to find, with computational efficiency, equilibria between the "identification related players" and the "data recovery players". These two parts are known to pose many challenges, from a theoretical point of view, like the identifiability issue, and from a numerical one, like convergence, stability and robustness problems. These questions are tricky [30] and still completely open for systems like e.g. coupled heat and thermoelastic joint data and material detection.

ANJA Team

3. Research Program

3.1. Research Program

The aim of Anja is to develop mathematical models in selected areas of SHS, which include, at this time, economy/finance, law, and archaeology. These models are essentially probabilistic. This entails that our theoretical studies mainly lie in the fields of probability and statistics.

A major focus of Anja is on providing mathematical analyses of how performativity operates in economy/finance and law, where performativity is understood as the phenomenon by which applying models co-constructs a new reality by the very fact that the existing reality was not properly apprehended. We are chiefly concerned with performativity that results from mathematical models. Indeed, while performativity exists before and independently of such models, mathematics may, and already have, strengthened the performative power in a significant way. This has occurred so far in a uncontrolled fashion, and thus in a typically damaging way. The essence of our work is to shed light on the mechanisms mediating the increase of performativity brought by mathematical models, thus allowing one to manage their effects and hopefully orient them towards an improvement of the reality they transform.

We stress the important fact that this program allows us to go well beyond what is typically achieved in sociological studies. For instance, many such studies have evidenced the role of performativity in the context of financial theory and how it shapes today's markets [46]. This is certainly useful in order to exert political control on the tools proposed by, e.g., economists. However, such an exogenous control is not fully satisfactory because it does not provide explicit procedures to enhance the models. This is due to the fact that these studies have not permeated the technical literature to a point where it would have a significant impact on the definition and practical use of models. One explanation for this is that, though convincing, these analyses do not provide mathematical or otherwise applicable tools to modify practices: they explain general mechanisms through which, for instance, economics performs the reality of economies, but do not shed light on the precise mathematics that mediate these mechanisms. We believe that it is important that mathematicians tackle this issue. In other words, we think that it is extremely useful to reverse that statement made in [48]: *"en souscrivant au programme de la performativité, la recherche en sociologie économique ne se contente plus de partager ses objets d'études avec les sciences économiques, elle inclut ces dernières dans ses propres objets d'étude"* [0]. Our "reverse" statement is that economical sciences, and, more generally, mathematics applied in SHS, should include in their research objectives the sociological impact they create through performativity: mathematicians need to take into account in their models the fact that reality will be transformed by them, and thus model also this transformation.

The first goal of Anja is precisely to fill this gap, that is, to pinpoint which parts of a given mathematical model are responsible for performative effects and how this occurs. It is important to stress that, in our view, this means that the performativity of mathematical models will be itself assessed with mathematical tools. This endogeneisation permits to measure quantitatively the impact of models on reality. In turn, this quantification opens the way to our second and more ambitious goal: indeed, we propose paradigms allowing one to control the performativity of mathematical models. The main mechanisms we use in that view are as follows:

- systematically take into account the fact that the models will perform reality. This means that, when defining our models, we try as much as possible to foresee how applying them will transform practices, and then adjust them in such a way that these modifications are desirable and under control;

[0] "By subscribing to the performativity program, research in economical sociology goes beyond sharing its objects of study with economical sciences: it includes the latter in its own objects of study.

- impose that the output of our models always be *probability distributions* rather than hard prescriptions. In other words, recognizing that modelling in SHS, in addition to being typically extremely complex with a large number of variables and with many sources of errors in the process of calibrating the parameters, always involves addressing a moving reality that will be transformed by the very application of the model, we insist that, at all stages of the analysis, *uncertainties* be propagated, as is routinely done in industrial fields such as aeronautics, so that the answer of the system will be probabilistic. We use in particular Bayesian analysis in that view, in order to incorporate information on unknown parameters using prior probability distributions that are sequentially updated after the acquisition of each new observation.

As a longer term perspective, we intend to propose a general mathematical model of performativity. The current literature has already proposed general analyses of mechanisms through which theories can become performative: most notably, [35] has identified three main such channels, namely institutional design, social norms, and language, as well as the way in which culture and accountability affect their course of operation. Our aim will be more focused: we will concentrate on the sole performativity of mathematical models, but in this restricted frame, we wish to propose quantitative, mathematical analyses. In other words, a mathematical model of performativity should allow one to answer questions such as: when can one expect that a theory is likely to be performative, what exactly are the conditions favouring performativity, which indices should one look for in order to detect a performative influence, how can one predict whether performativity will be convergent or divergent, which aspects of reality a theory will affect and how, and finally what are the means to minimize its negative effects.

One important motivation of Anja is that we feel that, as researchers in mathematics, we are partly responsible for the way mathematics is used in social sciences. In particular, while we strongly believe that mathematical models have already and will continue to enhance our social lives as they have improved our understanding and control in natural sciences, extra caution is needed because of their performative power explained above. The core of our work is that such caution can be exercised (a) by recognizing that models impact reality and by taking into account their performative power in their very definition, and (b) by using systematically probability and statistics: in a nutshell, imposing that mathematical answers to questions in social sciences always take the form of a probability distribution should (1) remind users that no mathematical model is able to provide a definitive hard and fast answer when it comes, e.g., to computing the amount of a fine in competition law, and (2) allow one to tame the inherent complexity of human-related matters, thus providing useful guides for making informed decisions.

Of course, we do not address performativity issues in all social and human sciences. Rather, we focus on two domains where we already have an expertise: economy/finance, and law. Details on our studies in these fields are given in sections 4.1 and 4.2 .

Our program cannot be realistically realised without strong collaborations from specialists in the SHS fields we deal with. In law, our expertise is brought by Jérôme Dupré, which holds a Ph.D. in law and is also a former judge. As far as archaeologyis concerned, we collaborate with Philippe Lanos (senior researcher at CNRS). He is an expert in archaeomagnetism and its applications to materials dating in archaeology.

APICS Project-Team

3. Research Program

3.1. Introduction

Within the extensive field of inverse problems, much of the research by Apics deals with reconstructing solutions of classical elliptic PDEs from their boundary behavior. Perhaps the simplest example lies with harmonic identification of a stable linear dynamical system: the transfer-function f can be evaluated at a point $i\omega$ of the imaginary axis from the response to a periodic input at frequency ω. Since f is holomorphic in the right half-plane, it satisfies there the Cauchy-Riemann equation $\overline{\partial} f = 0$, and recovering f amounts to solve a Dirichlet problem which can be done in principle using, *e.g.* the Cauchy formula.

Practice is not nearly as simple, for f is only measured pointwise in the pass-band of the system which makes the problem ill-posed [70]. Moreover, the transfer function is usually sought in specific form, displaying the necessary physical parameters for control and design. For instance if f is rational of degree n, then $\overline{\partial} f = \sum_1^n a_j \delta_{z_j}$ where the z_j are its poles and δ_{z_j} is a Dirac unit mass at z_j. Thus, to find the domain of holomorphy (*i.e.* to locate the z_j) amounts to solve a (degenerate) free-boundary inverse problem, this time on the left half-plane. To address such questions, the team has developed a two-step approach as follows.

> **Step 1:** To determine a complete model, that is, one which is defined at every frequency, in a sufficiently versatile function class (*e.g.* Hardy spaces). This ill-posed issue requires regularization, for instance constraints on the behavior at non-measured frequencies.
>
> **Step 2:** To compute a reduced order model. This typically consists of rational approximation of the complete model obtained in step 1, or phase-shift thereof to account for delays. We emphasize that deriving a complete model in step 1 is crucial to achieve stability of the reduced model in step 2.

Step 1 relates to extremal problems and analytic operator theory, see Section 3.3.1 . Step 2 involves optimization, and some Schur analysis to parametrize transfer matrices of given Mc-Millan degree when dealing with systems having several inputs and outputs, see Section 3.3.2.2 . It also makes contact with the topology of rational functions, in particular to count critical points and to derive bounds, see Section 3.3.2 . Step 2 raises further issues in approximation theory regarding the rate of convergence and the extent to which singularities of the approximant (*i.e.* its poles) tend to singularities of the approximated function; this is where logarithmic potential theory becomes instrumental, see Section 3.3.3 .

Applying a realization procedure to the result of step 2 yields an identification procedure from incomplete frequency data which was first demonstrated in [76] to tune resonant microwave filters. Harmonic identification of nonlinear systems around a stable equilibrium can also be envisaged by combining the previous steps with exact linearization techniques from [33].

A similar path can be taken to approach design problems in the frequency domain, replacing the measured behavior by some desired behavior. However, describing achievable responses in terms of the design parameters is often cumbersome, and most constructive techniques rely on specific criteria adapted to the physics of the problem. This is especially true of filters, the design of which traditionally appeals to polynomial extremal problems [72], [56]. Apics contributed to this area the use of Zolotarev-like problems for multi-band synthesis, although we presently favor interpolation techniques in which parameters arise in a more transparent manner, see Section 3.2.2 .

The previous example of harmonic identification quickly suggests a generalization of itself. Indeed, on identifying $\mathbb{C}$ with $\mathbb{R}^2$, holomorphic functions become conjugate-gradients of harmonic functions, so that harmonic identification is, after all, a special case of a classical issue: to recover a harmonic function on a domain from partial knowledge of the Dirichlet-Neumann data; when the portion of boundary where data are not available is itself unknown, we meet a free boundary problem. This framework for 2-D non-destructive control was first advocated in [61] and subsequently received considerable attention. It makes clear how to state similar problems in higher dimensions and for more general operators than the Laplacian, provided solutions are essentially determined by the trace of their gradient on part of the boundary which is the case for elliptic equations [0] [13], [79]. Such questions are particular instances of the so-called inverse potential problem, where a measure μ has to be recovered from the knowledge of the gradient of its potential (*i.e.*, the field) on part of a hypersurface (a curve in 2-D) encompassing the support of μ. For Laplace's operator, potentials are logarithmic in 2-D and Newtonian in higher dimensions. For elliptic operators with non constant coefficients, the potential depends on the form of fundamental solutions and is less manageable because it is no longer of convolution type. Nevertheless it is a useful concept bringing perspective on how problems could be raised and solved, using tools from harmonic analysis.

Inverse potential problems are severely indeterminate because infinitely many measures within an open set produce the same field outside this set; this phenomenon is called *balayage* [69]. In the two steps approach previously described, we implicitly removed this indeterminacy by requiring in step 1 that the measure be supported on the boundary (because we seek a function holomorphic throughout the right half-space), and by requiring in step 2 that the measure be discrete in the left half-plane (in fact: a sum of point masses $\sum_1^n a_j \delta_{z_j}$). The discreteness assumption also prevails in 3-D inverse source problems, see Section 4.3 . Conditions that ensure uniqueness of the solution to the inverse potential problem are part of the so-called regularizing assumptions which are needed in each case to derive efficient algorithms.

To recap, the gist of our approach is to approximate boundary data by (boundary traces of) fields arising from potentials of measures with specific support. This differs from standard approaches to inverse problems, where descent algorithms are applied to integration schemes of the direct problem; in such methods, it is the equation which gets approximated (in fact: discretized).

Along these lines, Apics advocates the use of steps 1 and 2 above, along with some singularity analysis, to approach issues of nondestructive control in 2-D and 3-D [2], [5], [40]. The team is currently engaged in the generalization to inverse source problems for the Laplace equation in 3-D, to be described further in Section 3.2.1 . There, holomorphic functions are replaced by harmonic gradients; applications are to EEG/MEG and inverse magnetization problems in geosciences, see Section 4.3 .

The approximation-theoretic tools developed by Apics to handle issues mentioned so far are outlined in Section 3.3 . In Section 3.2 to come, we describe in more detail which problems are considered and which applications are targeted.

3.2. Range of inverse problems

3.2.1. Elliptic partial differential equations (PDE)

Participants: Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Konstantinos Mavreas, Christos Papageorgakis, Dmitry Ponomarev.

By standard properties of conjugate differentials, reconstructing Dirichlet-Neumann boundary conditions for a function harmonic in a plane domain, when these conditions are already known on a subset E of the boundary, is equivalent to recover a holomorphic function in the domain from its boundary values on E. This is the problem raised on the half-plane in step 1 of Section 3.1 . It makes good sense in holomorphic Hardy spaces where functions are entirely determined by their values on boundary subsets of positive linear measure, which is the framework for Problem (P) that we set up in Section 3.3.1 . Such issues naturally arise in nondestructive testing of 2-D (or 3-D cylindrical) materials from partial electrical measurements on the boundary. For instance, the ratio between the tangential and the normal currents (the so-called Robin coefficient) tells one about corrosion of the material. Thus, solving Problem (P) where ψ is chosen to be the response of some uncorroded piece with identical shape yields non destructive testing of a potentially

[0] There is a subtle difference here between dimension 2 and higher. Indeed, a function holomorphic on a plane domain is defined by its non-tangential limit on a boundary subset of positive linear measure, but there are non-constant harmonic functions in the 3-D ball, C^1 up to the boundary sphere, yet having vanishing gradient on a subset of positive measure of the sphere. Such a "bad" subset, however, cannot have interior points on the sphere.

corroded piece of material, part of which is inaccessible to measurements. This was an initial application of holomorphic extremal problems to non-destructive control [54], [57].

Another application by the team deals with non-constant conductivity over a doubly connected domain, the set E being now the outer boundary. Measuring Dirichlet-Neumann data on E, one wants to recover level lines of the solution to a conductivity equation, which is a so-called free boundary inverse problem. For this, given a closed curve inside the domain, we first quantify how constant the solution on this curve. To this effect, we state and solve an analog of Problem (P), where the constraint bears on the real part of the function on the curve (it should be close to a constant there), in a Hardy space of a conjugate Beltrami equation, of which the considered conductivity equation is the compatibility condition (just like the Laplace equation is the compatibility condition of the Cauchy-Riemann system). Subsequently, a descent algorithm on the curve leads one to improve the initial guess. For example, when the domain is regarded as separating the edge of a tokamak's vessel from the plasma (rotational symmetry makes this a 2-D situation), this method can be used to estimate the shape of a plasma subject to magnetic confinement. This was actually carried out in collaboration with CEA (French nuclear agency) and the University of Nice (JAD Lab.), to data from *Tore Supra* [60]. The procedure is fast because no numerical integration of the underlying PDE is needed, as an explicit basis of solutions to the conjugate Beltrami equation in terms of Bessel functions was found in this case. Generalizing this approach in a more systematic manner to free boundary problems of Bernoulli type, using descent algorithms based on shape-gradient for such approximation-theoretic criteria, is an interesting prospect now under study in the team..

The piece of work we just mentioned requires defining and studying Hardy spaces of the conjugate-Beltrami equation, which is an interesting topic by itself. For Sobolev-smooth coefficients of exponent greater than 2, they were investigated in [4], [34]. The case of the critical exponent 2 is treated in [12], which apparently provides the first example of well-posedness for the Dirichlet problem in the non-strictly elliptic case: the conductivity may be unbounded or zero on sets of zero capacity and, accordingly, solutions need not be locally bounded. Exponent 2 seems also to be the key to a similar theory on general (rectifiable) domains in the plane, for exponent 2 is all one is left with in general after a conformal transformation of the domain.

Generalized Hardy classes as above are used in [13] where we address the uniqueness issue in the classical Robin inverse problem on a Lipschitz domain of $\Omega \subset \mathbb{R}^n$, $n \geq 2$, with uniformly bounded Robin coefficient, L^2 Neumann data and conductivity of Sobolev class $W^{1,r}(\Omega)$, $r > n$. We show that uniqueness of the Robin coefficient on a subset of the boundary, given Cauchy data on the complementary part, does hold in dimension $n = 2$, thanks to a unique continuation result, but needs not hold in higher dimension. In higher dimension, this raises an open issue on harmonic gradients, namely whether the positivity of the Robin coefficient is compatible with identical vanishing of the boundary gradient on a subset of positive measure.

The 3-D version of step 1 in Section 3.1 is another subject investigated by Apics: to recover a harmonic function (up to an additive constant) in a ball or a half-space from partial knowledge of its gradient. This prototypical inverse problem (*i.e.* inverse to the Cauchy problem for the Laplace equation) often recurs in electromagnetism. At present, Apics is involved with solving instances of this inverse problem arising in two fields, namely medical imaging *e.g.* for electroencephalography (EEG) or magneto-encephalography (MEG), and paleomagnetism (recovery of rocks magnetization) [2], [36], see Section 5.1 . In this connection, we collaborate with two groups of partners: Athena Inria project-team, CHU La Timone, and BESA company on the one hand, Geosciences Lab. at MIT and Cerege CNRS Lab. on the other hand. The question is considerably more difficult than its 2-D counterpart, due mainly to the lack of multiplicative structure for harmonic gradients. Still, substantial progress has been made over the last years using methods of harmonic analysis and operator theory.

The team is further concerned with 3-D generalizations and applications to non-destructive control of step 2 in Section 3.1 . A typical problem is here to localize inhomogeneities or defaults such as cracks, sources or occlusions in a planar or 3-dimensional object, knowing thermal, electrical, or magnetic measurements on the boundary. These defaults can be expressed as a lack of harmonicity of the solution to the associated Dirichlet-Neumann problem, thereby posing an inverse potential problem in order to recover them. In 2-D, finding an optimal discretization of the potential in Sobolev norm amounts to solve a best rational approximation problem, and the question arises as to how the location of the singularities of the approximant (*i.e.* its poles) reflects the location of the singularities of the potential (*i.e.* the defaults we seek). This is a fairly deep issue in approximation theory, to which Apics contributed convergence results for certain classes of fields expressed as Cauchy integrals over extremal contours for the logarithmic potential [6], [37], [51]. Initial schemes to locate cracks or sources *via* rational approximation on planar domains were obtained this way [40], [44], [54]. It is remarkable that finite inverse source problems in 3-D balls, or more general algebraic surfaces, can be approached using these 2-D techniques upon slicing the domain into planar sections [7], [41]. More precisely, each section cuts out a planar domain, the boundary of which carries data which can be proved to match an algebraic function. The singularities of this algebraic function are not located at the 3-D sources, but are related to them: the section contains a source if and only if some function of the singularities in that section meets a relative extremum. Using bisection it is thus possible to determine an extremal place along all sections parallel to a given plane direction, up to some threshold which has to be chosen small enough that one does not miss a source. This way, we reduce the original source problem in 3-D to a sequence of inverse poles and branchpoints problems in 2-D. This bottom line generates a steady research activity within Apics, and again applications are sought to medical imaging and geosciences, see Sections 4.3 , 4.2 and 5.1 .

Conjectures may be raised on the behavior of optimal potential discretization in 3-D, but answering them is an ambitious program still in its infancy.

3.2.2. Systems, transfer and scattering

Participants: Laurent Baratchart, Matthias Caenepeel, Sylvain Chevillard, Martine Olivi, Fabien Seyfert.

Through contacts with CNES (French space agency), members of the team became involved in identification and tuning of microwave electromagnetic filters used in space telecommunications, see Section 4.4 . The initial problem was to recover, from band-limited frequency measurements, physical parameters of the device under examination. The latter consists of interconnected dual-mode resonant cavities with negligible loss, hence its scattering matrix is modeled by a 2×2 unitary-valued matrix function on the frequency line, say the imaginary axis to fix ideas. In the bandwidth around the resonant frequency, a modal approximation of the Helmholtz equation in the cavities shows that this matrix is approximately rational, of Mc-Millan degree twice the number of cavities.

This is where system theory comes into play, through the so-called *realization* process mapping a rational transfer function in the frequency domain to a state-space representation of the underlying system of linear differential equations in the time domain. Specifically, realizing the scattering matrix allows one to construct a virtual electrical network, equivalent to the filter, the parameters of which mediate in between the frequency response and the geometric characteristics of the cavities (*i.e.* the tuning parameters).

Hardy spaces provide a framework to transform this ill-posed issue into a series of regularized analytic and meromorphic approximation problems. More precisely, the procedure sketched in Section 3.1 goes as follows:

1. infer from the pointwise boundary data in the bandwidth a stable transfer function (*i.e.* one which is holomorphic in the right half-plane), that may be infinite dimensional (numerically: of high degree). This is done by solving a problem analogous to (P) in Section 3.3.1 , while taking into account prior knowledge on the decay of the response outside the bandwidth, see [9] for details.
2. A stable rational approximation of appropriate degree to the model obtained in the previous step is performed. For this, a descent method on the compact manifold of inner matrices of given size and degree is used, based on an original parametrization of stable transfer functions developed within the team [28], [9].
3. Realizations of this rational approximant are computed. To be useful, they must satisfy certain constraints imposed by the geometry of the device. These constraints typically come from the coupling topology of the equivalent electrical network used to model the filter. This network is composed of resonators, coupled according to some specific graph. This realization step can be recast, under appropriate compatibility conditions [55], as solving a zero-dimensional multivariate polynomial system. To tackle this problem in practice, we use Gröbner basis techniques and continuation methods which team up in the Dedale-HF software (see Section 3.4.1).

Let us mention that extensions of classical coupling matrix theory to frequency-dependent (reactive) couplings have been carried-out in recent years [1] for wide-band design applications.

Apics also investigates issues pertaining to design rather than identification. Given the topology of the filter, a basic problem in this connection is to find the optimal response subject to specifications that bear on rejection, transmission and group delay of the scattering parameters. Generalizing the classical approach based on Chebyshev polynomials for single band filters, we recast the problem of multi-band response synthesis as a generalization of the classical Zolotarev min-max problem for rational functions [27] [8]. Thanks to quasi-convexity, the latter can be solved efficiently using iterative methods relying on linear programming. These were implemented in the software easy-FF (see easy-FF). Currently, the team is engaged in the synthesis of more complex microwave devices like multiplexers and routers, which connect several filters through wave guides. Schur analysis plays an important role here, because scattering matrices of passive systems are of Schur type (*i.e.* contractive in the stability region). The theory originates with the work of I. Schur [75], who devised a recursive test to check for contractivity of a holomorphic function in the disk. The so-called Schur parameters of a function may be viewed as Taylor coefficients for the hyperbolic metric of the disk, and the fact that Schur functions are contractions for that metric lies at the root of Schur's test. Generalizations thereof turn out to be efficient to parametrize solutions to contractive interpolation problems [29]. Dwelling on this, Apics contributed differential parametrizations (atlases of charts) of lossless matrix functions [28], [71], [65] which are fundamental to our rational approximation software RARL2 (see Section 3.4.4). Schur analysis is also instrumental to approach de-embedding issues, and provides one with considerable insight into the so-called matching problem. The latter consists in maximizing the power a multiport can pass to a given load, and for reasons of efficiency it is all-pervasive in microwave and electric network design, *e.g.* of antennas, multiplexers, wifi cards and more. It can be viewed as a rational approximation problem in the hyperbolic metric, and the team presently deals with this hot topic using contractive interpolation with constraints on boundary peak points, within the framework of the (defense funded) ANR COCORAM, see Sections 5.2 and 7.2.1 .

In recent years, our attention was driven by CNES and UPV (Bilbao) to questions about stability of high-frequency amplifiers, see Section 6.2 . Contrary to previously discussed devices, these are *active* components. The response of an amplifier can be linearized around a set of primary current and voltages, and then admittances of the corresponding electrical network can be computed at various frequencies, using the so-called harmonic balance method. The initial goal is to check for stability of the linearized model, so as to ascertain existence of a well-defined working state. The network is composed of lumped electrical elements namely inductors, capacitors, negative *and* positive reactors, transmission lines, and controlled current sources. Our research so far has focused on describing the algebraic structure of admittance functions, so as to set up a function-theoretic framework where the two-steps approach outlined in Section 3.1 can be put to work. The main discovery is that the unstable part of each partial transfer function is rational and can be computed by analytic projection, see Section 5.4 . We now start investigating the linearized harmonic transfer-function around a periodic cycle, to check for stability under non necessarily small inputs. This generalization generates both doctoral and postdoctoral work by new students in the team.

3.3. Approximation

Participants: Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Martine Olivi, Dmitry Ponomarev, Fabien Seyfert.

3.3.1. Best analytic approximation

In dimension 2, the prototypical problem to be solved in step 1 of Section 3.1 may be described as: given a domain $D \subset \mathbb{R}^2$, to recover a holomorphic function from its values on a subset K of the boundary of D. For the discussion it is convenient to normalize D, which can be done by conformal mapping. So, in the simply connected case, we fix D to be the unit disk with boundary unit circle T. We denote by H^p the Hardy space of exponent p, which is the closure of polynomials in $L^p(T)$-norm if $1 \leq p < \infty$ and the space of bounded holomorphic functions in D if $p = \infty$. Functions in H^p have well-defined boundary values in $L^p(T)$, which makes it possible to speak of (traces of) analytic functions on the boundary.

To find an analytic function g in D matching some measured values f approximately on a sub-arc K of T, we formulate a constrained best approximation problem as follows.

> (P) Let $1 \le p \le \infty$, K a sub-arc of T, $f \in L^p(K)$, $\psi \in L^p(T \setminus K)$ and $M > 0$; find a function $g \in H^p$ such that $\|g - \psi\|_{L^p(T \setminus K)} \le M$ and $g - f$ is of minimal norm in $L^p(K)$ under this constraint.

Here ψ is a reference behavior capturing *a priori* assumptions on the behavior of the model off K, while M is some admissible deviation thereof. The value of p reflects the type of stability which is sought and how much one wants to smooth out the data. The choice of L^p classes is suited to handle pointwise measurements.

To fix terminology, we refer to (P) as a *bounded extremal problem*. As shown in [39], [42], [48], the solution to this convex infinite-dimensional optimization problem can be obtained when $p \neq 1$ upon iterating with respect to a Lagrange parameter the solution to spectral equations for appropriate Hankel and Toeplitz operators. These spectral equations involve the solution to the special case $K = T$ of (P), which is a standard extremal problem [63]:

> (P_0) Let $1 \le p \le \infty$ and $\varphi \in L^p(T)$; find a function $g \in H^p$ such that $g - \varphi$ is of minimal norm in $L^p(T)$.

The case $p = 1$ is more or less open.

Various modifications of (P) can be tailored to meet specific needs. For instance when dealing with lossless transfer functions (see Section 4.4), one may want to express the constraint on $T \setminus K$ in a pointwise manner: $|g - \psi| \le M$ a.e. on $T \setminus K$, see [43]. In this form, the problem comes close to (but still is different from) H^∞ frequency optimization used in control [66], [74]. One can also impose bounds on the real or imaginary part of $g - \psi$ on $T \setminus K$, which is useful when considering Dirichlet-Neumann problems, see [68].

The analog of Problem (P) on an annulus, K being now the outer boundary, can be seen as a means to regularize a classical inverse problem occurring in nondestructive control, namely to recover a harmonic function on the inner boundary from Dirichlet-Neumann data on the outer boundary (see Sections 3.2.1 , 4.3 , 5.1.5). It may serve as a tool to approach Bernoulli type problems, where we are given data on the outer boundary and we *seek the inner boundary*, knowing it is a level curve of the solution. In this case, the Lagrange parameter indicates how to deform the inner contour in order to improve data fitting. Similar topics are discussed in Section 3.2.1 for more general equations than the Laplacian, namely isotropic conductivity equations of the form $\mathrm{div}(\sigma \nabla u) = 0$ where σ is no longer constant. Then, the Hardy spaces in Problem (P) are those of a so-called conjugate Beltrami equation: $\overline{\partial} f = \nu \overline{\partial f}$ [67], which are studied for $1 < p < \infty$ in [4], [12], [34] and [58]. Expansions of solutions needed to constructively handle such issues in the specific case of linear fractional conductivities (occurring for instance in plasma shaping) have been expounded in [60].

Another instance of problem (P) in with $p = 2$ and additional pointwise interpolation constraints inside a simply connected domain (disk) D was studied and solved in [11], Part I, and [15]. Such pointwise interpolation constraints could be of practical interest for inverse Cauchy type problems in cases where interior information is also available or to model uncertainty on boundary data.

Though originally considered in dimension 2, Problem (P) carries over naturally to higher dimensions where analytic functions get replaced by gradients of harmonic functions. Namely, given some open set $\Omega \subset \mathbb{R}^n$ and some $\mathbb{R}^n$-valued vector field V on an open subset O of the boundary of Ω, we seek a harmonic function in Ω whose gradient is close to V on O.

When Ω is a ball or a half-space, a substitute for holomorphic Hardy spaces is provided by the Stein-Weiss Hardy spaces of harmonic gradients [77]. Conformal maps are no longer available when $n > 2$, so that Ω can no longer be normalized. More general geometries than spheres and half-spaces have not been much studied so far.

On the ball, the analog of Problem (P) is

> (P_1) Let $1 \le p \le \infty$ and $B \subset \mathbb{R}^n$ the unit ball. Fix O an open subset of the unit sphere $S \subset \mathbb{R}^n$. Let further $V \in L^p(O)$ and $W \in L^p(S \setminus O)$ be $\mathbb{R}^n$-valued vector fields. Given $M > 0$, find a

harmonic gradient $G \in H^p(B)$ such that $\|G - W\|_{L^p(S \setminus O)} \leq M$ and $G - V$ is of minimal norm in $L^p(O)$ under this constraint.

When $p = 2$, Problem (P_1) was solved in [2] as well as its analog on a shell, when the tangent component of V is a gradient (when O is Lipschitz the general case follows easily from this). The solution extends the work in [39] to the 3-D case, using a generalization of Toeplitz operators. The case of the shell was motivated by applications to the processing of EEG data. An important ingredient is a refinement of the Hodge decomposition, that we call the *Hardy-Hodge* decomposition, allowing us to express a $\mathbb{R}^n$-valued vector field in $L^p(S)$, $1 < p < \infty$, as the sum of a vector field in $H^p(B)$, a vector field in $H^p(\mathbb{R}^n \setminus \overline{B})$, and a tangential divergence free vector field on S; the space of such divergence-free fields is denoted by $D(S)$. If $p = 1$ or $p = \infty$, L^p must be replaced by the real Hardy space or the space of functions with bounded mean oscillation. More generally this decomposition, which is valid on any sufficiently smooth surface (see Section 5.1), seems to play a fundamental role in inverse potential problems. In fact, it was first introduced formally on the plane to describe silent magnetizations supported in $\mathbb{R}^2$ (*i.e.* those generating no field in the upper half space) [36].

Just like solving problem (P) appeals to the solution of problem (P_0), our ability to solve problem (P_1) will depend on the possibility to tackle the special case where $O = S$:

> (P_2) Let $1 \leq p \leq \infty$ and $V \in L^p(S)$ be a $\mathbb{R}^n$-valued vector field. Find a harmonic gradient $G \in H^p(B)$ such that $\|G - V\|_{L^p(S)}$ is minimum.

Problem (P_2) is simple when $p = 2$ by virtue of the Hardy Hodge decomposition together with orthogonality of $H^2(B)$ and $H^2(\mathbb{R}^n \setminus \overline{B})$, which is the reason why we were able to solve (P_1) in this case. Other values of p cannot be treated as easily and are still under investigation, especially the case $p = \infty$ which is of particular interest and presents itself as a 3-D analog to the Nehari problem [73].

Companion to problem (P_2) is problem (P_3) below.

> (P_3) Let $1 \leq p \leq \infty$ and $V \in L^p(S)$ be a $\mathbb{R}^n$-valued vector field. Find $G \in H^p(B)$ and $D \in D(S)$ such that $\|G + D - V\|_{L^p(S)}$ is minimum.

Note that (P_2) and (P_3) are identical in 2-D, since no non-constant tangential divergence-free vector field exists on T. It is no longer so in higher dimension, where both (P_2) and (P_3) arise in connection with inverse potential problems in divergence form, like source recovery in electro/magneto encephalography and paleomagnetism, see Sections 3.2.1 and 4.3 .

3.3.2. Best meromorphic and rational approximation

The techniques set forth in this section are used to solve step 2 in Section 3.2 and they are instrumental to approach inverse boundary value problems for the Poisson equation $\Delta u = \mu$, where μ is some (unknown) measure.

3.3.2.1. Scalar meromorphic and rational approximation

We put R_N for the set of rational functions with at most N poles in D. By definition, meromorphic functions in $L^p(T)$ are (traces of) functions in $H^p + R_N$.

A natural generalization of problem (P_0) is:

> (P_N) Let $1 \leq p \leq \infty$, $N \geq 0$ an integer, and $f \in L^p(T)$; find a function $g_N \in H^p + R_N$ such that $g_N - f$ is of minimal norm in $L^p(T)$.

Only for $p = \infty$ and f continuous is it known how to solve (P_N) in semi-closed form. The unique solution is given by AAK theory (named after Adamjan, Arov and Krein), which connects the spectral decomposition of Hankel operators with best approximation [73].

The case where $p = 2$ is of special importance for it reduces to rational approximation. Indeed, if we write the Hardy decomposition $f = f^+ + f^-$ where $f^+ \in H^2$ and $f^- \in H^2(\mathbb{C} \setminus \overline{D})$, then $g_N = f^+ + r_N$ where r_N is a best approximant to f^- from R_N in $L^2(T)$. Moreover, r_N has no pole outside D, hence it is a *stable* rational approximant to f^-. However, in contrast to the case where $p = \infty$, this best approximant may *not* be unique.

The former Miaou project (predecessor of Apics) designed a dedicated steepest-descent algorithm for the case $p = 2$ whose convergence to a *local minimum* is guaranteed; until now it seems to be the only procedure meeting this property. This gradient algorithm proceeds recursively with respect to N on a compactification of the parameter space [32]. Although it has proved to be effective in all applications carried out so far (see Sections 4.3 , 4.4), it is still unknown whether the absolute minimum can always be obtained by choosing initial conditions corresponding to *critical points* of lower degree (as is done by the RARL2 software, Section 3.4.4).

In order to establish global convergence results, Apics has undertaken a deeper study of the number and nature of critical points (local minima, saddle points...), in which tools from differential topology and operator theory team up with classical interpolation theory [45], [47]. Based on this work, uniqueness or asymptotic uniqueness of the approximant was proved for certain classes of functions like transfer functions of relaxation systems (*i.e.* Markov functions) [49] and more generally Cauchy integrals over hyperbolic geodesic arcs [52]. These are the only results of this kind. Research by Apics on this topic remained dormant for a while by reasons of opportunity, but revisiting the work [30] in higher dimension is a worthy and timely endeavor today. Meanwhile, an analog to AAK theory was carried out for $2 \leq p < \infty$ in [48]. Although not as effective computationally, it was recently used to derive lower bounds [3]. When $1 \leq p < 2$, problem (P_N) is still quite open.

A common feature to the above-mentioned problems is that critical point equations yield non-Hermitian orthogonality relations for the denominator of the approximant. This stresses connections with interpolation, which is a standard way to build approximants, and in many respects best or near-best rational approximation may be regarded as a clever manner to pick interpolation points. This was exploited in [53], [50], and is used in an essential manner to assess the behavior of poles of best approximants to functions with branched singularities, which is of particular interest for inverse source problems (*cf.* Sections 3.4.2 and 5.1).

In higher dimensions, the analog of Problem (P_N) is best approximation of a vector field by gradients of discrete potentials generated by N point masses. This basic issue is by no means fully understood, and it is an exciting field of research. It is connected with certain generalizations of Toeplitz or Hankel operators, and with constructive approaches to so-called weak factorizations for real Hardy functions [59].

Besides, certain constrained rational approximation problems, of special interest in identification and design of passive systems, arise when putting additional requirements on the approximant, for instance that it should be smaller than 1 in modulus (*i.e.* a Schur function). In particular, Schur interpolation lately received renewed attention from the team, in connection with matching problems. There, interpolation data are subject to a well-known compatibility condition (positive definiteness of the so-called Pick matrix), and the main difficulty is to put interpolation points on the boundary of D while controlling both the degree and the extremal points (peak points for the modulus) of the interpolant. Results obtained by Apics in this direction generalize a variant of contractive interpolation with degree constraint as studied in [64], see Section 5.2 . We mention that contractive interpolation with nodes approaching the boundary has been a subsidiary research topic by the team in the past, which plays an interesting role in the spectral representation of certain non-stationary stochastic processes [35], [38]. The subject is intimately connected to orthogonal polynomials on the unit circle, and this line of investigation has been pursued towards an asymptotic study of orthogonal polynomials on planar domains, which is today an active area in approximation theory with application to quantum particle systems, spectra of random matrices, and Hele-Shaw flows, see Section 5.6 .

3.3.2.2. Matrix-valued rational approximation

Matrix-valued approximation is necessary to handle systems with several inputs and outputs but it generates additional difficulties as compared to scalar-valued approximation, both theoretically and algorithmically. In the matrix case, the McMillan degree (*i.e.* the degree of a minimal realization in the System-Theoretic sense) generalizes the usual notion of degree for rational functions. For instance when poles are simple, the McMillan degree is the sum of the ranks of the residues.

The basic problem that we consider now goes as follows: *let $\mathcal{F} \in (H^2)^{m\times l}$ and n an integer; find a rational matrix of size $m \times l$ without poles in the unit disk and of McMillan degree at most n which is nearest possible* *to $\mathcal{F}$ in* $(H^2)^{m\times l}$. Here the L^2 norm of a matrix is the square root of the sum of the squares of the norms of its entries.

The scalar approximation algorithm derived in [32] and mentioned in Section 3.3.2.1 generalizes to the matrix-valued situation [62]. The first difficulty here is to parametrize inner matrices (*i.e.* matrix-valued functions analytic in the unit disk and unitary on the unit circle) of given McMillan degree degree n. Indeed, inner matrices play the role of denominators in fractional representations of transfer matrices (using the so-called Douglas-Shapiro-Shields factorization). The set of inner matrices of given degree is a smooth manifold that allows one to use differential tools as in the scalar case. In practice, one has to produce an atlas of charts (local parametrizations) and to handle changes of charts in the course of the algorithm. Such parametrization can be obtained using interpolation theory and Schur-type algorithms, the parameters of which are vectors or matrices ([28], [65], [71]). Some of these parametrizations are also interesting to compute realizations and achieve filter synthesis ([65], [71]). The rational approximation software “RARL2” developed by the team is described in Section 3.4.4 .

Difficulties relative to multiple local minima of course arise in the matrix-valued case as well, and deriving criteria that guarantee uniqueness is even more difficult than in the scalar case. The case of rational functions of degree n or small perturbations thereof (the consistency problem) was solved in [46]. Matrix-valued Markov functions are the only known example beyond this one [31].

Let us stress that RARL2 seems the only algorithm handling rational approximation in the matrix case that demonstrably converges to a local minimum while meeting stability constraints on the approximant. It is still a working pin of many developments by Apics on frequency optimization and design.

3.3.3. Behavior of poles of meromorphic approximants

Participant: Laurent Baratchart.

We refer here to the behavior of poles of best meromorphic approximants, in the L^p-sense on a closed curve, to functions f defined as Cauchy integrals of complex measures whose support lies inside the curve. Normalizing the contour to be the unit circle T, we are back to Problem (P_N) in Section 3.3.2.1 ; invariance of the latter under conformal mapping was established in [5]. Research so far has focused on functions whose singular set inside the contour is polar, meaning that the function can be continued analytically (possibly in a multiple-valued manner) except over a set of logarithmic capacity zero.

Generally speaking in approximation theory, assessing the behavior of poles of rational approximants is essential to obtain error rates as the degree goes large, and to tackle constructive issues like uniqueness. However, as explained in Section 3.2.1 , the original twist by Apics is to consider this issue also as a means to extract information on singularities of the solution to a Dirichlet-Neumann problem. The general theme is thus: *how do the singularities of the approximant reflect those of the approximated function?* This approach to inverse problem for the 2-D Laplacian turns out to be attractive when singularities are zero- or one-dimensional (see Section 4.3). It can be used as a computationally cheap initial condition for more precise but much heavier numerical optimizations which often do not even converge unless properly initialized. As regards crack detection or source recovery, this approach boils down to analyzing the behavior of best meromorphic approximants of given pole cardinality to a function with branch points, which is the prototype of a polar singular set. For piecewise analytic cracks, or in the case of sources, we were able to prove ([5], [6], [37]), that the poles of the approximants accumulate, when the degree goes large, to some extremal cut of minimum weighted logarithmic capacity connecting the singular points of the crack, or the sources [40]. Moreover, the asymptotic density of the poles turns out to be the Green equilibrium distribution on this cut in D, therefore it charges the singular points if one is able to approximate in sufficiently high degree (this is where the method could fail, because high-order approximation requires rather precise data).

The case of two-dimensional singularities is still an outstanding open problem.

It is remarkable that inverse source problems inside a sphere or an ellipsoid in 3-D can be approached with such 2-D techniques, as applied to planar sections, see Section 5.1 . The technique is implemented in the software FindSources3D, see Section 3.4.2 .

3.4. Software tools of the team

In addition to the above-mentioned research activities, Apics develops and maintains a number of long-term software tools that either implement and illustrate effectiveness of the algorithms theoretically developed by the team or serve as tools to help further research by team members. We present briefly the most important of them.

3.4.1. DEDALE-HF

SCIENTIFIC DESCRIPTION

Dedale-HF consists in two parts: a database of coupling topologies as well as a dedicated predictor-corrector code. Roughly speaking each reference file of the database contains, for a given coupling topology, the complete solution to the coupling matrix synthesis problem (C.M. problem for short) associated to particular filtering characteristics. The latter is then used as a starting point for a predictor-corrector integration method that computes the solution to the C.M. corresponding to the user-specified filter characteristics. The reference files are computed off-line using Gröbner basis techniques or numerical techniques based on the exploration of a monodromy group. The use of such continuation techniques, combined with an efficient implementation of the integrator, drastically reduces the computational time.

Dedale-HF has been licensed to, and is currently used by TAS-Espana
FUNCTIONAL DESCRIPTION

Dedale-HF is a software dedicated to solve exhaustively the coupling matrix synthesis problem in reasonable time for the filtering community. Given a coupling topology, the coupling matrix synthesis problem consists in finding all possible electromagnetic coupling values between resonators that yield a realization of given filter characteristics. Solving the latter is crucial during the design step of a filter in order to derive its physical dimensions, as well as during the tuning process where coupling values need to be extracted from frequency measurements.

- Participant: Fabien Seyfert
- Contact: Fabien Seyfert
- URL: http://www-sop.inria.fr/apics/Dedale/

3.4.2. FindSources3D

FindSources3D-bolis
KEYWORDS: Health - Neuroimaging - Visualization - Compilers - Medical - Image - Processing
FUNCTIONAL DESCRIPTION

FindSources3D is a software program dedicated to the resolution of inverse source problems in electroencephalography (EEG). From pointwise measurements of the electrical potential taken by electrodes on the scalp, FindSources3D estimates pointwise dipolar current sources within the brain in a spherical model.

After a first data transmission "cortical mapping" step, it makes use of best rational approximation on 2-D planar cross-sections and of the software RARL2 in order to locate singularities. From those planar singularities, the 3-D sources are estimated in a last step.

This version of FindSources3D provides a modular, ergonomic, accessible and interactive platform, with a convenient graphical interface and a tool that can be distributed and used, for EEG medical imaging. Modularity is now granted (using the tools dtk, Qt, with compiled Matlab libraries). It offers a detailed and nice visualization of data and tuning parameters, processing steps, and of the computed results (using VTK).

- Participants: Juliette Leblond, Maureen Clerc Gallagher, Théodore Papadopoulo, Jean-Paul Marmorat and Nicolas Schnitzler
- Contact: Juliette Leblond
- URL: http://www-sop.inria.fr/apics/FindSources3D/en/index.html

3.4.3. PRESTO-HF

SCIENTIFIC DESCRIPTION

For the matrix-valued rational approximation step, Presto-HF relies on RARL2. Constrained realizations are computed using the Dedale-HF software. As a toolbox, Presto-HF has a modular structure, which allows one for example to include some building blocks in an already existing software.

The delay compensation algorithm is based on the following assumption: far off the pass-band, one can reasonably expect a good approximation of the rational components of S11 and S22 by the first few terms of their Taylor expansion at infinity, a small degree polynomial in 1/s. Using this idea, a sequence of quadratic convex optimization problems are solved, in order to obtain appropriate compensations. In order to check the previous assumption, one has to measure the filter on a larger band, typically three times the pass band.

This toolbox has been licensed to, and is currently used by Thales Alenia Space in Toulouse and Madrid, Thales airborne systems and Flextronics (two licenses). XLIM (University of Limoges) is a heavy user of Presto-HF among the academic filtering community and some free license agreements have been granted to the microwave department of the University of Erlangen (Germany) and the Royal Military College (Kingston, Canada).

FUNCTIONAL DESCRIPTION

Presto-HF is a toolbox dedicated to low-pass parameter identification for microwave filters. In order to allow the industrial transfer of our methods, a Matlab-based toolbox has been developed, dedicated to the problem of identification of low-pass microwave filter parameters. It allows one to run the following algorithmic steps, either individually or in a single stroke:

• Determination of delay components caused by the access devices (automatic reference plane adjustment),

• Automatic determination of an analytic completion, bounded in modulus for each channel,

• Rational approximation of fixed McMillan degree,

• Determination of a constrained realization.

- Participants: Fabien Seyfert, Jean-Paul Marmorat and Martine Olivi
- Contact: Fabien Seyfert
- URL: https://project.inria.fr/presto-hf/

3.4.4. RARL2

Réalisation interne et Approximation Rationnelle L2

SCIENTIFIC DESCRIPTION

The method is a steepest-descent algorithm. A parametrization of MIMO systems is used, which ensures that the stability constraint on the approximant is met. The implementation, in Matlab, is based on state-space representations.

RARL2 performs the rational approximation step in the software tools PRESTO-HF and FindSources3D. It is distributed under a particular license, allowing unlimited usage for academic research purposes. It was released to the universities of Delft and Maastricht (the Netherlands), Cork (Ireland), Brussels (Belgium), Macao (China) and BITS-Pilani Hyderabad Campus (India).

FUNCTIONAL DESCRIPTION

RARL2 is a software for rational approximation. It computes a stable rational L2-approximation of specified order to a given L2-stable (L2 on the unit circle, analytic in the complement of the unit disk) matrix-valued function. This can be the transfer function of a multivariable discrete-time stable system. RARL2 takes as input either:

• its internal realization,

• its first N Fourier coefficients,

• discretized (uniformly distributed) values on the circle. In this case, a least-square criterion is used instead of the L2 norm.

It thus performs model reduction in the first or the second case, and leans on frequency data identification in the third. For band-limited frequency data, it could be necessary to infer the behavior of the system outside the bandwidth before performing rational approximation.

An appropriate Möbius transformation allows to use the software for continuous-time systems as well.

- Participants: Jean-Paul Marmorat and Martine Olivi
- Contact: Martine Olivi
- URL: http://www-sop.inria.fr/apics/RARL2/rarl2.html

3.4.5. Sollya

KEYWORDS: Numerical algorithm - Supremum norm - Curve plotting - Remez algorithm - Code generator - Proof synthesis

FUNCTIONAL DESCRIPTION

Sollya is an interactive tool where the developers of mathematical floating-point libraries (libm) can experiment before actually developing code. The environment is safe with respect to floating-point errors, i.e. the user precisely knows when rounding errors or approximation errors happen, and rigorous bounds are always provided for these errors.

Among other features, it offers a fast Remez algorithm for computing polynomial approximations of real functions and also an algorithm for finding good polynomial approximants with floating-point coefficients to any real function. As well, it provides algorithms for the certification of numerical codes, such as Taylor Models, interval arithmetic or certified supremum norms.

It is available as a free software under the CeCILL-C license.

- Participants: Sylvain Chevillard, Christoph Lauter, Mioara Joldes and Nicolas Jourdan
- Partners: CNRS - ENS Lyon - UCBL Lyon 1
- Contact: Sylvain Chevillard
- URL: http://sollya.gforge.inria.fr/

ASPI Project-Team

3. Research Program

3.1. Interacting Monte Carlo methods and particle approximation of Feynman–Kac distributions

Monte Carlo methods are numerical methods that are widely used in situations where (i) a stochastic (usually Markovian) model is given for some underlying process, and (ii) some quantity of interest should be evaluated, that can be expressed in terms of the expected value of a functional of the process trajectory, which includes as an important special case the probability that a given event has occurred. Numerous examples can be found, e.g. in financial engineering (pricing of options and derivative securities) [43], in performance evaluation of communication networks (probability of buffer overflow), in statistics of hidden Markov models (state estimation, evaluation of contrast and score functions), etc. Very often in practice, no analytical expression is available for the quantity of interest, but it is possible to simulate trajectories of the underlying process. The idea behind Monte Carlo methods is to generate independent trajectories of this process or of an alternate instrumental process, and to build an approximation (estimator) of the quantity of interest in terms of the weighted empirical probability distribution associated with the resulting independent sample. By the law of large numbers, the above estimator converges as the size N of the sample goes to infinity, with rate $1/\sqrt{N}$ and the asymptotic variance can be estimated using an appropriate central limit theorem. To reduce the variance of the estimator, many variance reduction techniques have been proposed. Still, running independent Monte Carlo simulations can lead to very poor results, because trajectories are generated *blindly*, and only afterwards are the corresponding weights evaluated. Some of the weights can happen to be negligible, in which case the corresponding trajectories are not going to contribute to the estimator, i.e. computing power has been wasted.

A major breakthrough made in the mid 90's, has been the introduction of interacting Monte Carlo methods, also known as sequential Monte Carlo (SMC) methods, in which a whole (possibly weighted) sample, called *system of particles*, is propagated in time, where the particles

- *explore* the state space under the effect of a *mutation* mechanism which mimics the evolution of the underlying process,
- and are *replicated* or *terminated*, under the effect of a *selection* mechanism which automatically concentrates the particles, i.e. the available computing power, into regions of interest of the state space.

In full generality, the underlying process is a discrete–time Markov chain, whose state space can be

> finite, continuous, hybrid (continuous / discrete), graphical, constrained, time varying, pathwise, etc.,

the only condition being that it can easily be *simulated*.

In the special case of particle filtering, originally developed within the tracking community, the algorithms yield a numerical approximation of the optimal Bayesian filter, i.e. of the conditional probability distribution of the hidden state given the past observations, as a (possibly weighted) empirical probability distribution of the system of particles. In its simplest version, introduced in several different scientific communities under the name of *bootstrap filter* [45], *Monte Carlo filter* [49] or *condensation* (conditional density propagation) algorithm [48], and which historically has been the first algorithm to include a resampling step, the selection mechanism is governed by the likelihood function: at each time step, a particle is more likely to survive and to replicate at the next generation if it is consistent with the current observation. The algorithms also provide as a by–product a numerical approximation of the likelihood function, and of many other contrast functions for parameter estimation in hidden Markov models, such as the prediction error or the conditional least–squares criterion.

Particle methods are currently being used in many scientific and engineering areas

> positioning, navigation, and tracking [46], [39], visual tracking [48], mobile robotics [40], [61], ubiquitous computing and ambient intelligence, sensor networks, risk evaluation and simulation of rare events [44], genetics, molecular simulation [41], etc.

Other examples of the many applications of particle filtering can be found in the contributed volume [28] and in the special issue of *IEEE Transactions on Signal Processing* devoted to *Monte Carlo Methods for Statistical Signal Processing* in February 2002, where the tutorial paper [29] can be found, and in the textbook [56] devoted to applications in target tracking. Applications of sequential Monte Carlo methods to other areas, beyond signal and image processing, e.g. to genetics, can be found in [54]. A recent overview can also be found in [31].

Particle methods are very easy to implement, since it is sufficient in principle to simulate independent trajectories of the underlying process. The whole problematic is multidisciplinary, not only because of the already mentioned diversity of the scientific and engineering areas in which particle methods are used, but also because of the diversity of the scientific communities which have contributed to establish the foundations of the field

> target tracking, interacting particle systems, empirical processes, genetic algorithms (GA), hidden Markov models and nonlinear filtering, Bayesian statistics, Markov chain Monte Carlo (MCMC) methods.

These algorithms can be interpreted as numerical approximation schemes for Feynman–Kac distributions, a pathwise generalization of Gibbs–Boltzmann distributions, in terms of the weighted empirical probability distribution associated with a system of particles. This abstract point of view [36], [35], has proved to be extremely fruitful in providing a very general framework to the design and analysis of numerical approximation schemes, based on systems of branching and / or interacting particles, for nonlinear dynamical systems with values in the space of probability distributions, associated with Feynman–Kac distributions. Many asymptotic results have been proved as the number N of particles (sample size) goes to infinity, using techniques coming from applied probability (interacting particle systems, empirical processes [63]), see e.g. the survey article [36] or the textbooks [35], [34], and references therein

> convergence in $\mathbb{L}^p$, convergence as empirical processes indexed by classes of functions, uniform convergence in time, see also [52], [53], central limit theorem, see also [50], [37], propagation of chaos, large deviations principle, etc.

The objective here is to systematically study the impact of the many algorithmic variants on the convergence results.

3.2. Multilevel splitting for rare event simulation

See 4.2 , and 6.1 .

The estimation of the small probability of a rare but critical event, is a crucial issue in industrial areas such as

> nuclear power plants, food industry, telecommunication networks, finance and insurance industry, air traffic management, etc.

In such complex systems, analytical methods cannot be used, and naive Monte Carlo methods are clearly unefficient to estimate accurately very small probabilities. Besides importance sampling, an alternate widespread technique consists in multilevel splitting [51], where trajectories going towards the critical set are given offsprings, thus increasing the number of trajectories that eventually reach the critical set. As shown in [6], the Feynman–Kac formalism of 3.1 is well suited for the design and analysis of splitting algorithms for rare event simulation.

Propagation of uncertainty Multilevel splitting can be used in static situations. Here, the objective is to learn the probability distribution of an output random variable $Y = F(X)$, where the function F is only defined pointwise for instance by a computer programme, and where the probability distribution of the input random variable X is known and easy to simulate from. More specifically, the objective could be to compute the probability of the output random variable exceeding a threshold, or more generally to evaluate the cumulative distribution function of the output random variable for different output values. This problem is characterized by the lack of an analytical expression for the function, the computational cost of a single pointwise evaluation of the function, which means that the number of calls to the function should be limited as much as possible, and finally the complexity and / or unavailability of the source code of the computer programme, which makes any modification very difficult or even impossible, for instance to change the model as in importance sampling methods.

The key issue is to learn as fast as possible regions of the input space which contribute most to the computation of the target quantity. The proposed splitting methods consists in (i) introducing a sequence of intermediate regions in the input space, implicitly defined by exceeding an increasing sequence of thresholds or levels, (ii) counting the fraction of samples that reach a level given that the previous level has been reached already, and (iii) improving the diversity of the selected samples, usually with an artificial Markovian dynamics for the input variable. In this way, the algorithm learns

- the transition probability between successive levels, hence the probability of reaching each intermediate level,
- and the probability distribution of the input random variable, conditionned on the output variable reaching each intermediate level.

A further remark, is that this conditional probability distribution is precisely the optimal (zero variance) importance distribution needed to compute the probability of reaching the considered intermediate level.

Rare event simulation To be specific, consider a complex dynamical system modelled as a Markov process, whose state can possibly contain continuous components and finite components (mode, regime, etc.), and the objective is to compute the probability, hopefully very small, that a critical region of the state space is reached by the Markov process before a final time T, which can be deterministic and fixed, or random (for instance the time of return to a recurrent set, corresponding to a nominal behaviour).

The proposed splitting method consists in (i) introducing a decreasing sequence of intermediate, more and more critical, regions in the state space, (ii) counting the fraction of trajectories that reach an intermediate region before time T, given that the previous intermediate region has been reached before time T, and (iii) regenerating the population at each stage, through resampling. In addition to the non–intrusive behaviour of the method, the splitting methods make it possible to learn the probability distribution of typical critical trajectories, which reach the critical region before final time T, an important feature that methods based on importance sampling usually miss. Many variants have been proposed, whether

- the branching rate (number of offsprings allocated to a successful trajectory) is fixed, which allows for depth–first exploration of the branching tree, but raises the issue of controlling the population size,
- the population size is fixed, which requires a breadth–first exploration of the branching tree, with random (multinomial) or deterministic allocation of offsprings, etc.

Just as in the static case, the algorithm learns

- the transition probability between successive levels, hence the probability of reaching each intermediate level,
- and the entrance probability distribution of the Markov process in each intermediate region.

Contributions have been given to

- minimizing the asymptotic variance, obtained through a central limit theorem, with respect to the shape of the intermediate regions (selection of the importance function), to the thresholds (levels), to the population size, etc.

- controlling the probability of extinction (when not even one trajectory reaches the next intermediate level),
- designing and studying variants suited for hybrid state space (resampling per mode, marginalization, mode aggregation),

and in the static case, to

- minimizing the asymptotic variance, obtained through a central limit theorem, with respect to intermediate levels, to the Metropolis kernel introduced in the mutation step, etc.

A related issue is global optimization. Indeed, the difficult problem of finding the set M of global minima of a real–valued function V can be replaced by the apparently simpler problem of sampling a population from a probability distribution depending on a small parameter, and asymptotically supported by the set M as the small parameter goes to zero. The usual approach here is to use the cross–entropy method [57], [33], which relies on learning the optimal importance distribution within a prescribed parametric family. On the other hand, multilevel splitting methods could provide an alternate nonparametric approach to this problem.

3.3. Statistical learning: pattern recognition and nonparametric regression

In pattern recognition and statistical learning, also known as machine learning, nearest neighbor (NN) algorithms are amongst the simplest but also very powerful algorithms available. Basically, given a training set of data, i.e. an N–sample of i.i.d. object–feature pairs, with real–valued features, the question is how to generalize, that is how to guess the feature associated with any new object. To achieve this, one chooses some integer k smaller than N, and takes the mean–value of the k features associated with the k objects that are nearest to the new object, for some given metric.

In general, there is no way to guess exactly the value of the feature associated with the new object, and the minimal error that can be done is that of the Bayes estimator, which cannot be computed by lack of knowledge of the distribution of the object–feature pair, but the Bayes estimator can be useful to characterize the strength of the method. So the best that can be expected is that the NN estimator converges, say when the sample size N grows, to the Bayes estimator. This is what has been proved in great generality by Stone [58] for the mean square convergence, provided that the object is a finite–dimensional random variable, the feature is a square–integrable random variable, and the ratio k/N goes to 0. Nearest neighbor estimator is not the only local averaging estimator with this property, but it is arguably the simplest.

The asymptotic behavior when the sample size grows is well understood in finite dimension, but the situation is radically different in general infinite dimensional spaces, when the objects to be classified are functions, images, etc.

Nearest neighbor classification in infinite dimension In finite dimension, the k–nearest neighbor classifier is universally consistent, i.e. its probability of error converges to the Bayes risk as N goes to infinity, whatever the joint probability distribution of the pair, provided that the ratio k/N goes to zero. Unfortunately, this result is no longer valid in general metric spaces, and the objective is to find out reasonable sufficient conditions for the weak consistency to hold. Even in finite dimension, there are exotic distances such that the nearest neighbor does not even get closer (in the sense of the distance) to the point of interest, and the state space needs to be complete for the metric, which is the first condition. Some regularity on the regression function is required next. Clearly, continuity is too strong because it is not required in finite dimension, and a weaker form of regularity is assumed. The following consistency result has been obtained: if the metric space is separable and if some Besicovich condition holds, then the nearest neighbor classifier is weakly consistent. Note that the Besicovich condition is always fulfilled in finite dimensional vector spaces (this result is called the Besicovich theorem), and that a counterexample [4] can be given in an infinite dimensional space with a Gaussian measure (in this case, the nearest neighbor classifier is clearly nonconsistent). Finally, a simple example has been found which verifies the Besicovich condition with a noncontinuous regression function.

Rates of convergence of the functional k–nearest neighbor estimator Motivated by a broad range of potential applications, such as regression on curves, rates of convergence of the k–nearest neighbor estimator of the regression function, based on N independent copies of the object–feature pair, have been investigated when the object is in a suitable ball in some functional space. Using compact embedding theory, explicit and general finite sample bounds can be obtained for the expected squared difference between the k–nearest neighbor estimator and the Bayes regression function, in a very general setting. The results have also been particularized to classical function spaces such as Sobolev spaces, Besov spaces and reproducing kernel Hilbert spaces. The rates obtained are genuine nonparametric convergence rates, and up to our knowledge the first of their kind for k–nearest neighbor regression.

This topic has produced several theoretical advances [1], [2] in collaboration with Gérard Biau (université Pierre et Marie Curie). A few possible target application domains have been identified in

- the statistical analysis of recommendation systems,
- the design of reduced–order models and analog samplers,

that would be a source of interesting problems.

BIPOP Project-Team

3. Research Program

3.1. Dynamic non-regular systems

nonsmooth mechanical systems, impacts, friction, unilateral constraints, complementarity problems, modeling, analysis, simulation, control, convex analysis

Dynamical systems (we limit ourselves to finite-dimensional ones) are said to be *non-regular* whenever some nonsmoothness of the state arises. This nonsmoothness may have various roots: for example some outer impulse, entailing so-called *differential equations with measure*. An important class of such systems can be described by the complementarity system

$$\left\{\begin{array}{l} \dot{x} = f(x,u,\lambda)\,, \\ 0 \le y \perp \lambda \ge 0\,, \\ g(y,\lambda,x,u,t) = 0\,, \\ \text{re-initialization law of the state } x(\cdot), \end{array}\right. \tag{2}$$

where $\perp$ denotes orthogonality; u is a control input. Now (1) can be viewed from different angles.

- Hybrid systems: it is in fact natural to consider that (1) corresponds to different models, depending whether $y_i = 0$ or $y_i > 0$ (y_i being a component of the vector y). In some cases, passing from one mode to the other implies a jump in the state x; then the continuous dynamics in (1) may contain distributions.
- Differential inclusions: $0 \le y \perp \lambda \ge 0$ is equivalent to $-\lambda \in \mathrm{N}_K(y)$, where K is the nonnegative orthant and $\mathrm{N}_K(y)$ denotes the normal cone to K at y. Then it is not difficult to reformulate (1) as a differential inclusion.
- Dynamic variational inequalities: such a formalism reads as $\langle \dot{x}(t) + F(x(t),t), v - x(t)\rangle \ge 0$ for all $v \in K$ and $x(t) \in K$, where K is a nonempty closed convex set. When K is a polyhedron, then this can also be written as a complementarity system as in (1).

Thus, the 2nd and 3rd lines in (1) define the modes of the hybrid systems, as well as the conditions under which transitions occur from one mode to another. The 4th line defines how transitions are performed by the state x. There are several other formalisms which are quite related to complementarity. See [7], [8], [15] for a survey on models and control issues in nonsmooth mechanical systems.

3.2. Nonsmooth optimization

optimization, numerical algorPierre-Brice Wieber.ithm, convexity, Lagrangian relaxation, combinatorial optimization.

Here we are dealing with the minimization of a function f (say over the whole space R^n), whose derivatives are discontinuous. A typical situation is when f comes from dualization, if the primal problem is not strictly convex – for example a large-scale linear program – or even nonconvex – for example a combinatorial optimization problem. Also important is the case of spectral functions, where $f(x) = F(\lambda(A(x)))$, A being a symmetric matrix and λ its spectrum.

For these types of problems, we are mainly interested in developing efficient resolution algorithms. Our basic tool is bundling and we act along two directions:

- To explore application areas where nonsmooth optimization algorithms can be applied, possibly after some tayloring. A rich field of such application is combinatorial optimization, with all forms of relaxation.
- To explore the possibility of designing more sophisticated algorithms. This implies an appropriate generalization of second derivatives when the first derivative does not exist, and we use advanced tools of nonsmooth analysis.

$\Longrightarrow$*The optimization scientific activity in BIPOP is no longer existing after Jérôme Malick left BIPOP to lead the DAO team in the Laboratoire Jean Kuntzman.*

CAGIRE Project-Team

3. Research Program

3.1. The scientific context

3.1.1. Computational fluid mechanics: modeling or not before discretizing ?

A typical continuous solution of the Navier Stokes equations at sufficiently high values of the Reynolds number is governed by a spectrum of time and space scales fluctuations closely connected with the turbulent nature of the flow. The term deterministic chaos employed by Frisch in his enlightening book [42] is certainly conveying most adequately the difficulty in analyzing and simulating this kind of flows. The broadness of the turbulence spectrum is directly controlled by the Reynolds number defined as the ratio between the inertial forces and the viscous forces. This number is not only useful to determine the transition from a laminar to a turbulent flow regime, it also indicates the range of scales of fluctuations that are present in the flow under consideration. Typically, for the velocity field and far from solid walls, the ratio between the largest scale (the integral length scale) to the smallest one (Kolmogorov scale) scales as $Re^{3/4}$ per dimension. In addition, for internal flows, the viscous effects near the solid walls yield a scaling proportional to Re per dimension. The smallest scales play a crucial role in the dynamics of the largest ones which implies that an accurate framework for the computation of turbulent flows must take into account all these scales. Thus, the usual practice to deal with turbulent flows is to choose between an a priori modeling (in most situations) or not (low Re number and rather simple configurations) before proceeding to the discretization step followed by the simulation runs themselves. If a modeling phase is on the agenda, then one has to choose again among the above mentioned variety of approaches. As it is illustrated in Fig. 1 , this can be achieved either by directly solving the Navier-Stokes equations (DNS) or by first applying a statistical averaging (RANS) or a spatial filtering operator to the Navier-Stokes equations (LES). The new terms brought about by the filtering operator have to be modeled. From a computational point of view, the RANS approach is the least demanding, which explains why historically it has been the workhorse in both the academic and the industrial sectors. It has permitted quite a substantial progress in the understanding of various phenomena such as turbulent combustion or heat transfer. Its inherent inability to provide a time-dependent information has led to promote in the last decade the recourse to either LES or DNS to supplement if not replace RANS. By simulating the large scale structures while modeling the smallest ones supposed to be more isotropic, LES proved to be quite a step through that permits to fully take advantage of the increasing power of computers to study complex flow configurations. At the same time, DNS was progressively applied to geometries of increasing complexity (channel flows with values of Re_τ multiplied by 10 during the last 15 years, jets, turbulent premixed flames, among many others), and proved to be a formidable tool that permits **(i)** to improve our knowledge on turbulent flows and **(ii)** to test (i.e., validate or invalidate) and improve the modeling hypotheses inherently associated to the RANS and LES approaches. From a numerical point of view, if the steady nature of the RANS equations allows to perform iterative convergence on finer and finer meshes, the high computational cost of LES or DNS makes necessary the use of highly accurate numerical schemes in order to optimize the use of computational resources. To the noticeable exception of the hybrid RANS-LES modeling, which is not yet accepted as a reliable tool for industrial design, as mentioned in the preamble of the Go4hybrid European program [0], once chosen, a single turbulence model will (try to) do the job for modeling the whole flow. Thus, depending on its intrinsic strengths and weaknesses, the accuracy will be a rather volatile quantity strongly dependent on the flow configuration. The turbulence modeling and industrial design communities waver between the desire to continue to rely on the RANS approach, which is unrivaled in terms of computational cost, but is still not able to accurately represent all the complex phenomena; and the temptation to switch to LES, which outperforms RANS in many situations but is prohibitively expensive in high-Reynolds number wall-bounded flows. In order to account for the deficiencies of both approaches and to combine them for significantly improving the overall quality of

[0] http://www.transport-research.info/web/projects/project_details.cfm?id=46810

the modeling, the hybrid RANS-LES approach has emerged during the last decade as a viable, intermediate way, and we are definitely inscribing our project in this innovative field of research, with an original approach though, connected with a time filtered hybrid RANS-LES and a systematic and progressive validation process against experimental data produced by the team.

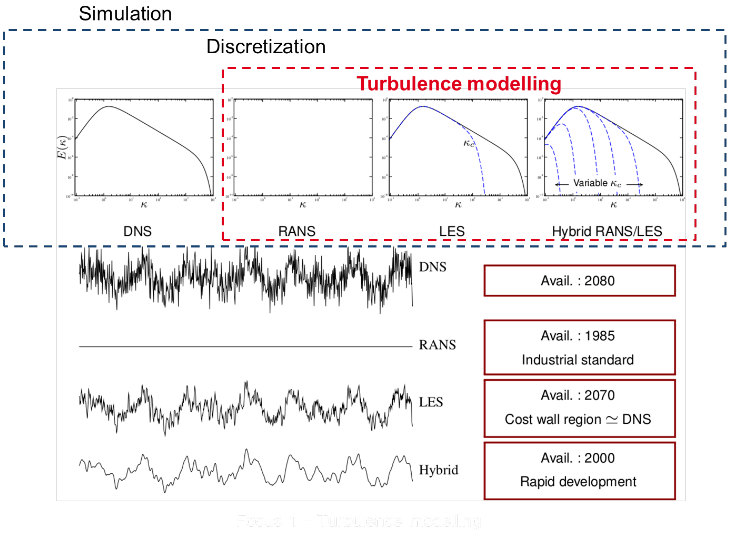


Figure 1. A schematic view of the different nested steps for turbulent flow simulation: from DNS to hybrid RANS-LES. The approximate dates at which the different approaches are or will be routinely used in the industry are indicated in the boxes on the right (extrapolations based on the present rate of increase in computer performances).

3.1.2. Computational fluid mechanics: high order discretization on unstructured meshes and efficient methods of solution

All the methods considered in the project are mesh-based methods: the computational domain is divided into cells, that have an elementary shape: triangles and quadrangles in two dimensions, and tetrahedra, hexahedra, pyramids, and prisms in three dimensions. If the cells are only regular hexahedra, the mesh is said to be structured. Otherwise, it is said to be unstructured. If the mesh is composed of more than one sort of elementary shape, the mesh is said to be hybrid. In the project, the numerical strategy is based on discontinuous Galerkin methods. These methods were introduced by Reed and Hill [53] and first studied by Lesaint and Raviart [49]. The extension to the Euler system with explicit time integration was mainly led by Shu, Cockburn and their collaborators. The steps of time integration and slope limiting were similar to high order ENO schemes, whereas specific constraints given by the finite element nature of the scheme were progressively solved, for scalar conservation laws [38], [37], one dimensional systems [36], multidimensional scalar conservation laws [35], and multidimensional systems [39]. For the same system, we can also cite the work of [41], [46], which is slightly different: the stabilization is made by adding a nonlinear term, and the time integration is implicit. Contrary to continuous Galerkin methods, the discretization of diffusive operators is not straightforward. This is due to the discontinuous approximation space, which does not fit well with the space function in which the diffusive system is well posed. A first stabilization was proposed by Arnold [28]. The first application of discontinuous Galerkin methods to Navier-Stokes equations was proposed in [33] by mean of a mixed formulation. Actually, this first attempt led to a non compact computation stencil, and was later proved to be not stable. A compactness improvement was made in [34], which was later analyzed, and proved to be stable in a more unified framework [29]. The combination with the $k - \omega$ RANS model was made in [32]. As far as Navier Stokes equations are concerned, we can also cite the work of [44], in which the stabilization is closer to the one of [29], the work of [50] on local time stepping, or the first use of discontinuous Galerkin methods for direct numerical simulation of a turbulent channel flow done in [40]. Discontinuous Galerkin methods are so popular because:

- They can be developed for any order of approximation.
- The computational stencil of one given cell is limited to the cells with which it has a common face. This stencil does not depend on the order of approximation. This is a pro, compared for example with high order finite volumes, which require as more and more neighbors as the order increases.
- They can be developed for any kind of mesh, structured, unstructured, but also for aggregated grids [31]. This is a pro compared not only with finite differences schemes, which can be developed only on structured meshes, but also compared with continuous finite elements methods, for which the definition of the approximation basis is not clear on aggregated elements.
- p-adaptivity is easier than with continuous finite elements, because neighboring elements having a different order are only weakly coupled.
- Upwinding is as natural as for finite volumes methods, which is a benefit for hyperbolic problems.
- As the formulation is weak, boundary conditions are naturally weakly formulated. This is a benefit compared with strong formulations, for example point centered formulation when a point is at the intersection of two kinds of boundary conditions.

For concluding this section, there already exist numerical schemes based on the discontinuous Galerkin method which proved to be efficient for computing compressible viscous flows. Nevertheless, there remain many things to be improved, which include: efficient shock capturing methods for supersonic flows, high order discretization of curved boundaries, low Mach number behavior of these schemes and combination with second-moment RANS models.Another drawback of the discontinuous Galerkin methods is that they can be computationally costly, due to the accurate representation of the solution calling for a particular care of implementation for being efficient. We believe that this cost can be balanced by the strong memory locality of the method, which is an asset for porting on emerging many-core architectures.

3.1.3. Experimental fluid mechanics: a relevant tool for physical modeling and simulation development

With the considerable and constant development of computer performance, many people were thinking at the turn of the 21st century that in the short term, CFD would replace experiments considered as too costly and not flexible enough. Simply flipping through scientific journals such as Journal of Fluid Mechanics, Combustion of Flame, Physics of Fluids or Journal of Computational Physics or through websites such that of Ercoftac [0] is sufficient to convince oneself that the recourse to experiments to provide either a quantitative description of complex phenomena or reference values for the assessment of the predictive capabilities of the physical modeling and of the related simulations is still necessary. The major change that can be noted though concerns the content of the interaction between experiments and CFD (understood in the broad sense). Indeed, LES or DNS assessment calls for the experimental determination of time and space turbulent scales as well as time resolved measurements and determination of single or multi-point statistical properties of the velocity field. Thus, the team methodology incorporates from the very beginning an experimental component that is operated in strong interaction with the physical modeling and the simulation activities.

3.2. Research directions

3.2.1. Boundary conditions

3.2.1.1. Generating synthetic turbulence

[0] http://www.ercoftac.org

A crucial point for any multi-scale simulation able to locally switch (in space or time) from a coarse level of turbulence description to a more refined one, is the enrichment of the solution by fluctuations as physically meaningful as possible. Basically, this issue is an extension of the problem of the generation of realistic inlet boundary conditions in DNS or LES of subsonic turbulent flows. In that respect, the method of anisotropic linear forcing (ALF) we have developed in collaboration with EDF proved very encouraging, by its efficiency, its generality and simplicity of implementation. So, it seems natural, on the one hand, to extend this approach to the compressible framework and then implement it in AeroSol. On the other hand, we shall concentrate (in cooperation with EDF R&D in Chatou via a CIFRE PhD do be started next year) on the theoretical link between the local variations of the scale's description of turbulence (e.g. a sudden variations in the size of the time filter) and the intensity of the ALF forcing transiently applied to help in the development of missing scales of fluctuations.

3.2.1.2. Stable and non reflecting boundary conditions

In aerodynamics, and especially for subsonic computations, handling inlet and outlet boundary conditions is a difficult issue. A lot of work has already been done for second order schemes for Navier Stokes equations, see [52], [55] and the huge number of papers citing it. On the one hand, we believe that strong improvements are necessary with higher order schemes: indeed, the less dissipative the scheme is, the worse impact have the spurious reflections. For this, we will first concentrate on the linearized Navier-Stokes system, and analyze the boundary condition imposition in a discontinuous Galerkin framework with a similar approach as in [43]. We will also try to extend the work of [56], which deals with Euler equations, to the Navier Stokes equations.

3.2.2. Turbulence models and model agility

3.2.2.1. Extension of zero Mach models to the compressible system

We shall develop in parallel our multi-scale turbulence modeling and the related adaptive numerical methods of AeroSol. Without prejudice to methods that will be on the podium in the future, a first step in this direction will be to extend to a compressible framework the continuous hybrid temporal RANS/LES models we have developed up to now in a Mach zero context.

3.2.2.2. Study of wall flows with and without mass or heat transfer at the wall: determination and validation of relevant criteria for hybrid turbulence models

In the targeted application domains, the turbulence/wall interaction and the heat transfer at the fluid-solid interfaces are physical phenomena whose numerical prediction is at the heart of the concerns of our industrial partners. For instance, for a jet engine manufacturer, being able to properly design the configuration of the cooling of the walls of its engine combustion chamber in the presence of thermoacoustic instabilities is based on the proper identification and a thorough understanding of the major mechanisms that drive the dynamics of the parietal transfers. For our part, we will gradually use all our analysis and experimentation tools to actively participate in the improvement of the collective knowledge on such kind of transfers. The flow configurations dealt with by the beginning of the project will be those of subsonic single phase impacting jets or JICF with the possible presence of an interacting acoustic wave. The conjugate heat transfer at the wall will be also progressively tackled. The existing criteria of switching of the hybrid RANS/LES model will be tested on those flow configurations in order to determine their domain of validity. In parallel, the hydrodynamic instability modes of the JICF will be studied experimentally and theoretically (in cooperation with the SIAME laboratory) in order to determine if it is possible to drive a change of instability regime (e.g. from absolute to convective) and so propose challenging flow conditions that would be relevant for the setting-up of an hybrid LES/DNS approach aimed at supplementing the hybrid RANS/LES one.

3.2.2.3. Improvement of turbulence models

The production and the subsequent use of DNS (AeroSol library) and experimental (bench MAVERIC) databases dedicated to the improvement of the physical models will be an important part of our activity. In that respect, our present capability of producing in-situ experimental data for simulation validation and flow analysis is clearly a strongly differentiating mark of our project. It is on the improvement of the hybrid RANS/LES approach that will focus most of our initial efforts of analysis of the DNS and experimental data as soon as they will become available. This method has a decisive advantage over all other hybrid

RANS/LES approaches since it relies on a well defined time filtering formalism. This greatly facilitates the proper extraction from the databases of the various terms appearing in the relevant flux balances obtained at the different scales involved (e.g. from RANS to LES). But we would not be comprehensive in that matter if we were not questioning the relevance of any simulation-experiment comparisons. In other words, a central issue will also be to answer positively the following question: will we be comparing the same quantities between simulations and experiment? From an experimental point of view, the questions to be raised will be, among others, the possible difference in resolution between the experiment and the simulations, the similar location of the measurement points and simulation points, the acceptable level of random error associated to the necessary finite number of samples. In that respect, the recourse to uncertainty quantification techniques will be advantageously considered.

3.2.3. Development of an efficient implicit high-order compressible solver scalable on new architectures

As the flows we wish to simulate may be very computationally demanding, we will maintain our efforts in the development of AeroSol in the following directions:

- Efficient implementation of the discontinuous Galerkin method.
- Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid.
- Porting on heterogeneous architectures.
- Implementation of models.

3.2.3.1. Efficient implementation of the discontinuous Galerkin method

In high order discontinuous Galerkin methods, the unknown vector is composed of a concatenation of the unknowns in the cells of the mesh. An explicit residual computation is composed of three loops: an integration loop on the cells, for which computations in two different cells are independent, an integration loop on boundary faces, in which computations depend on data of one cell and on the boundary conditions, and an integration loop on the interior faces, in which computations depend on data of the two neighboring cells. Each of these loops are composed of three steps: the first step consists in interpolating data at the quadrature points, the second step in computing a nonlinear flux at the quadrature points (the physical flux for the cell loop, an upwind flux for interior faces or a flux adapted to the kind of boundary condition for boundary faces), and the third step consists in projecting the nonlinear flux on the degrees of freedom.

In this research direction, we propose to exploit the strong memory locality of the method (i.e., the fact that all the unknowns of a cell are stocked contiguously). This formulation can reduce the linear steps of the method (interpolation on the quadrature points and projection on the degrees of freedom) to simple matrix-matrix product which can be optimized. For the nonlinear steps, composed of the computation of the physical flux on the cells and of the numerical flux on the faces, we will try to exploit vectorization.

3.2.3.2. Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid

For our computations of the IMPACT-AE project, we use an explicit time stepping. The time stepping is limited by the CFL condition, and in our flow, the time step is limited by the acoustic wave velocity. As the Mach number of the flow we simulate in IMPACT-AE is low, the acoustic time restriction is much lower than the turbulent time scale, which is driven by the velocity of the flow. We hope to have a better efficiency by using time implicit methods, for using a time step driven by the velocity of the flow.

Using implicit time stepping in compressible flows in particularly difficult, because the system is fully nonlinear, so that the nonlinear solving theoretically requires to build many times the Jacobian. Our experience in implicit methods is that the building of a Jacobian is very costly, especially in three dimensions and in a high order framework, because the optimization of the memory usage is very difficult. That is why we propose to use Jacobian free implementation, based on [48]. This method consists in solving the linear steps of the Newton method by a Krylov method, which requires Jacobian-vector product. The smart idea of this method is to replace this product by an approximation based on a difference of residual, therefore avoiding any Jacobian computation. Nevertheless, Krylov methods are known to converge slowly, especially for the compressible system when the Mach number is low, because the system is ill-conditioned. In order to precondition, we propose to use an aggregation-based multigrid method, which consists in using the same numerical method on coarser meshes obtained by aggregation of the initial mesh. This choice is driven by the fact that multigrid methods are the only one to scale linearly [57], [58] with the number of unknowns in term of number of operations, and that this preconditioning does not require any Jacobian computation.

Beyond the technical aspects of the multigrid approach, which will be challenging to implement, we are also interested in the design of an efficient aggregation. This often means to perform an aggregation based on criteria (anisotropy of the problem, for example) [51]. For this, we propose to extend the scalar analysis of [59] to a linearized version of the Euler and Navier-Stokes equations, and try to deduce an optimal strategy for anisotropic aggregation, based on the local characteristics of the flow. Note that discontinuous Galerkin methods are particularly well suited to h-p aggregation, as this kind of methods can be defined on any shape [31].

3.2.3.3. Porting on heterogeneous architectures

Until the beginning of the 2000s, the computing capacities have been improved by interconnecting an increasing number of more and more powerful computing nodes. The computing capacity of each node was increased by improving the clock speed, the number of cores per processor, the introduction of a separate and dedicated memory bus per processor, but also the instruction level parallelism, and the size of the memory cache. Even if the number of transistors kept on growing up, the clock speed improvement has flattened since the mid 2000s [54]. Already in 2003, [45] pointed out the difficulties for efficiently using the biggest clusters: "While these super-clusters have theoretical peak performance in the Teraflops range, sustained performance with real applications is far from the peak. Salinas, one of the 2002 Gordon Bell Awards was able to sustain 1.16 Tflops on ASCI White (less than 10% of peak)." From the current multi-core architectures, the trend is now to use many-core accelerators. The idea behind many-core is to use an accelerator composed of a lot of relatively slow and simplified cores for executing the most simple parts of the algorithm. The larger the part of the code executed on the accelerator, the faster the code may become. In this task, we will work on the heterogeneous aspects of computation. These heterogeneities are intrinsic to our computations and have two sources. The first one is the use of hybrid meshes, which are necessary for using a local structured mesh in a boundary layer. As the different cell shapes (pyramids, hexahedra, prisms and tetrahedra) do not have the same number of degrees of freedom, nor the same number of quadrature points, the execution time on one face or one cell depends on its shape. The second source of heterogeneity are the boundary conditions. Depending on the kind of boundary conditions, user defined boundary values might be needed, which induces a different computational cost. Heterogeneities are typically what may decrease efficiency in parallel if the workload is not well balanced between the cores. Note that heterogeneities were not dealt with in what we consider as one of the most advanced work on discontinuous Galerkin on GPU [47], as only straight simplicial cell shapes were addressed. For managing at best our heterogeneous computations on heterogeneous architectures, we propose to use the execution runtime StarPU [30]. For this, the discontinuous Galerkin algorithm will be reformulated in term of a graph of tasks. The previous tasks on the memory management will be useful for that. The linear steps of the discontinuous Galerkin methods require also memory transfers, and one task of the project will consist in determining the optimal task granularity for this step, i.e. the number of cells or face integrations to be sent in parallel on the accelerator. On top of that, the question of which device is the most appropriate to tackle such kind of tasks will be discussed.

Last, we point out that the combination of shared-memory and distributed-memory parallel programming models is better suited than only the distributed-memory one for multigrid, because in a hybrid version, a wider part of the mesh shares the same memory, therefore allowing for a coarser aggregation.

The consortium will benefit from a particularly stimulating environment in the Inria Bordeaux Sud Ouest center around high performance computing, which is one of the strategic axis of the center.

3.2.3.4. Implementation of turbulence models in AeroSol and validation

We will gradually insert models developed in research direction 3.2.2.1 in the AeroSol library in which we develop methods for the DNS of compressible turbulent flows at low Mach number. Indeed, thanks to its formalism of temporal filtering, the HTLES approach offers a theoretical framework characterized by a continuous transition from RANS to DNS, even for complex flow configurations (e.g. without directions of spatial homogeneity). As for the discontinuous Galerkin method available presently in AeroSol, it is the best suited and versatile method able to meet the requirements of accuracy, stability and cost related to the local (varying) level of resolution of the turbulent flow at hand, regardless of its configuration complexity. This task is part of a the European project iHybrid, coordinated by TU Berlin, that we are currently writting in collaboration with two of our industrial partners, EDF and PSA.

3.2.4. Validation of the simulations: test flow configurations

To supplement whenever necessary the test flow configuration of MAVERIC and apart from configurations that could emerge in the course of the project, the following configurations for which either experimental data, simulation data or both have been published will be used whenever relevant for benchmarking the quality of our agile computations:

- The impinging turbulent jet (simulations).
- The ORACLES two-channel dump combustor developed in the European projects LES4LPP and MOLECULES.
- The non reactive single-phase PRECCINSTA burner (monophasic swirler), a configuration that has been extensively calculated in particular with the AVBP and Yales2 codes.
- The LEMCOTEC configuration (monophasic swirler + effusion cooling).
- The ONERA MERCATO two-phase injector configuration provided the question of confidentiality of the data is not an obstacle.
- Rotating turbulent flows with wall interaction and heat transfer.
- Turbulent flows with buoyancy.

CARDAMOM Project-Team

3. Research Program

3.1. Variational discrete asymptotic modelling

In many of the applications we consider, intermediate fidelity models are or can be derived using an asymptotic expansion for the relevant scale resolving PDEs, and eventually considering some averaged for of the resulting continuous equations. The resulting systems of PDEs are often very complex and their characterization, e.g. in terms of stability, unclear, or poor, or too complex to allow to obtain discrete analogy of the continuous properties. This makes the numerical approximation of these PDE systems a real challenge. Moreover, most of these models are often based on asymptotic expansions involving small geometrical scales. This is true for many applications considered here involving flows in/of thin layers (free surface waves, liquid films on wings generating ice layers, oxide flows in material cracks, etc). This asymptotic expansion is nothing else than a discretization (some sort of Taylor expansion) in terms of the small parameter. The actual discretization of the PDE system is another expansion in space involving as a small parameter the mesh size. What is the interaction between these two expansions ? Could we use the spatial discretization (truncation error) as means of filtering undesired small scales instead of having to explicitly derive PDEs for the large scales ? We will investigate in depth the relations between asymptotics and discretization by :

- comparing the asymptotic limits of discretized forms of the relevant scale resolving equations with the discretization of the analogous continuous asymptotic PDEs. Can we discretize a well understood system of PDEs instead of a less understood and more complex one ? ;
- study the asymptotic behaviour of error terms generated by coarse one-dimensional discretization in the direction of the “small scale”. What is the influence of the number of cells along the vertical direction, and of their clustering ? ;
- derive equivalent continuous equations (modified equations) for anisotropic discretizations in which the direction is direction of the “small scale” is approximated with a small number of cells. What is the relation with known asymptotic PDE systems ?

Our objective is to gain sufficient control of the interaction between discretization and asymptotics to be able to replace the coupling of several complex PDE systems by adaptive strongly anisotrotropic finite element approximations of relevant and well understood PDEs. Here the anisotropy is intended in the sense of having a specific direction in which a much poorer (and possibly variable with the flow conditions) polynomial approximation (expansion) is used. The final goal is, profiting from the availability of faster and cheaper computational platforms, to be able to automatically control numerical *and* physical accuracy of the model with the same techniques. This activity will be used to improve our modelling in coastal engineering as well as for de-anti icing systems, wave energy converters, composite materials (cf. next sections).

In parallel to these developments, we will make an effort in to gain a better understanding of continuous asymptotic PDE models. We will in particular work on improving, and possibly, simplifying their numerical approximation. An effort will be done in trying to embed in these more complex nonlinear PDE models discrete analogs of operator identities necessary for stability (see e.g. the recent work of [106], [110] and references therein).

3.2. High order discretizations on moving adaptive meshes

We will work on both the improvement of high order mesh generation and adaptation techniques, and the construction of more efficient, adaptive high order discretisation methods.

Concerning curved mesh generation, we will focus on two points. First propose a robust and automatic method to generate curved simplicial meshes for realistic geometries. The untangling algorithm we plan to develop is a hybrid technique that gathers a local mesh optimization applied on the surface of the domain and a linear elasticity analogy applied in its volume. Second we plan to extend the method proposed in [60] to hybrid meshes (prism/tetra).

For time dependent adaptation we will try to exploit as much as possible the use of $r-$adaptation techniques based on the solution of some PDE system for the mesh. We will work on enhancing the initial results of [64], [66] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [120], [127], [76]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [60], and with improved algorithms to discretize accurately and fast the elliptic equations involved. For this we will explore different type of relaxation methods, including those proposed in [107], [113], [112] allowing to re-use high order discretizations techniques already used for the flow variables. All these modelling approaches for the mesh movement are based on some minimization argument, and do not allow easily to take into account explicitly properties such as e.g. the positivity of nodal volumes. An effort will be made to try to embed these properties, as well as to improve the control on the local mesh sizes obtained. Developments made in numerical methods for Lagrangian hydrodynamics and compressible materials may be a possible path for these objectives (see e.g. [86], [133], [132] and references therein). We will stretch the use of these techniques as much as we can, and couple them with remeshing algorithms based on local modifications plus conservative, high order, and monotone ALE (or other) remaps (cf. [61], [96], [134], [84] and references therein).

The development of high order schemes for the discretization of the PDE will be a major part of our activity. We will work from the start in an Arbitrary Lagrangian Eulerian setting, so that mesh movement will be easily accommodated, and investigate the following main points:

- the ALE formulation is well adapted both to handle moving meshes, and to provide conservative, high order, and monotone remaps between different meshes. We want to address the issue of cost-accuracy of adaptive mesh computations by exploring different degrees of coupling between the flow and the mesh PDEs. Initial experience has indicated that a clever coupling may lead to a considerable CPU time reduction for a given resolution [66], [64]. This balance is certainly dependent on the nature of the PDEs, on the accuracy level sought, on the cost of the scheme, and on the time stepping technique. All these elements will be taken into account to try to provide the most efficient formulation ;
- the conservation of volume, and the subsequent preservation of constant mass-momentum-energy states on deforming domains is one of the most primordial elements of Arbitrary Lagrangian-Eulerian formulations. For complex PDEs as the ones considered here, of especially for some applications, there may be a competition between the conservation of e.g. mass, an the conservation of other constant states, as important as mass. This is typically the case for free surface flows, in which mass preservation is in competitions with the preservation of constant free surface levels [65]. Similar problems may arise in other applications. Possible solutions to this competition may come from super-approximation (use of higher order polynomials) of some of the data allowing to reduce (e.g. bathymetry) the error in the preservation of one of the competing quantities. This is similar to what is done in super-parametric approximations of the boundaries of an object immersed in the flow, except that in our case the data may enter the PDE explicitly and not only through the boundary conditions. Several efficient solutions for this issue will be investigated to obtain fully conservative moving mesh approaches:
- an issue related to the previous one is the accurate treatment of wall boundaries. It is known that even for standard lower order (second) methods, a higher order, curved, approximation of the boundaries may be beneficial. This, however, may become difficult when considering moving objects, as in the case e.g. of the study of the impact of ice debris in the flow. To alleviate this issue, we plan to follow on with our initial work on the combined use of immersed boundaries techniques with high order, anisotropic (curved) mesh adaptation. In particular, we will develop combined approaches involving high order hybrid meshes on fixed boundaries with the use of penalization techniques and immersed

boundaries for moving objects. We plan to study the accuracy obtainable across discontinuous functions with $r-$adaptive techniques, and otherwise use whenever necessary anisotropic meshes to be able to provide a simplified high order description of the wall boundary (cf. [105]). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body [111], [114]. An effort will be also made on improving the accuracy of these techniques using e.g. higher order approaches, either based on generalizations of classical splitting methods [97], or on some iterative Defect Correction method (see e.g. [78]) ;

- the proper treatment of different physics may be addressed by using mixed/hybrid schemes in which different variables/equations are approximated using a different polynomial expansion. A typical example is our work on the discretization of highly non-linear wave models [92] in which we have shown how to use a standard continuous Galerkin method for the elliptic equation/variable representative of the dispersive effects, while the underlying hyperbolic system is evolved using a (discontinuous) third order finite volume method. This technique will be generalized to other classes of discontinuous methods, and similar ideas will be used in other context to provide a flexible approximation. Such mathods have clear advantages in multiphase flows but not only. A typical example where such mixed methods are beneficial are flows involving different species and tracer equations, which are typically better treated with a discontinuous approximation. Another example is the use of this mixed approximation to describe the topography with a high order continuous polynomial even in discontinuous method. This allows to greatly simplify the numerical treatment of the bathymetric source terms ;
- the enhancement of stabilized methods based on some continuous finite element approximation will remain a main topic. We will further pursue the study on the construction of simplified stabilization operators which do not involve any contributions to the mass matrix. We will in particular generalize our initial results [122], [63], [123] to higher order spatial approximations using cubature points, or Bezier polynomials, or also hierarchical approximations. This will also be combined with time dependent variants of the reconstruction techniques initially proposed by D. Caraeni [77], allowing to have a more flexible approach similar to the so-called $\mathrm{P^nP^m}$ method [89], [126]. How to localize these enhancements, and to efficiently perform local reconstructions/enrichment, as well as $p-$adaptation, and handling hanging nodes will also be a main line of work. A clever combination of hierarchical enrichment of the polynomials, with a constrained approximation will be investigated. All these developments will be combined with the shock capturing/positivity preserving construction we developed in the past. Other discontinuity resolving techniques will be investigated as well, such as face limiting techniques as those partially studied in [94] ;
- time stepping is an important issue, especially in presence of local mesh adaptation. The techniques we use will force us to investigate local and multilevel techniques. We will study the possibility constructing semi-implicit methods combining extrapolation techniques with space-time variational approaches. Other techniques will be considered, as multi-stage type methods obtained using Defect-Correction, Multi-step Runge-Kutta methods [74], as well as spatial partitioning techniques [102]. A major challenge will be to be able to guarantee sufficient locality to the time integration method to allow to efficiently treat highly refined meshes, especially for viscous reactive flows. Another challenge will be to embed these methods in the stabilized methods we will develop.

3.3. Coupled approximation/adaptation in parameter and physical space

As already remarked, classical methods for uncertainty quantification are affected by the so-called Curse-of-Dimensionality. Adaptive approaches proposed so far, are limited in terms of efficiency, or of accuracy. Our aim here is to develop methods and algorithms permitting a very high-fidelity simulation in the physical and in the stochastic space at the same time. We will focus on both non-intrusive and intrusive approaches.

Simple non-intrusive techniques to reduce the overall cost of simulations under uncertainty will be based on adaptive quadrature in stochastic space with mesh adaptation in physical space using error monitors related to the variance of to the sensitivities obtained e.g. by an ANOVA decomposition. For steady state problems, remeshing using metric techniques is enough. For time dependent problems both mesh deformation and remeshing techniques will be used. This approach may be easily used in multiple space dimensions to minimize the overall cost of model evaluations by using high order moments of the properly chosen output functional for the adaptation (as in optimization). Also, for high order curved meshes, the use of high order moments and sensitivities issued from the UQ method or optimization provides a viable solution to the lack of error estimators for high order schemes.

Despite the coupling between stochastic and physical space, this approach can be made massively parallel by means of extrapolation/interpolation techniques for the high order moments, in time and on a reference mesh, guaranteeing the complete independence of deterministic simulations. This approach has the additional advantage of being feasible for several different application codes due to its non-intrusive character.

To improve on the accuracy of the above methods, intrusive approaches will also be studied. To propagate uncertainties in stochastic differential equations, we will use Harten's multiresolution framework, following [59]. This framework allows a reduction of the dimensionality of the discrete space of function representation, defined in a proper stochastic space. This reduction allows a reduction of the number of explicit evaluations required to represent the function, and thus a gain in efficiency. Moreover, multiresolution analysis offers a natural tool to investigate the local regularity of a function and can be employed to build an efficient refinement strategy, and also provides a procedure to refine/coarsen the stochastic space for unsteady problems. This strategy should allow to capture and follow all types of flow structures, and, as proposed in [59], allows to formulate a non-linear scheme in terms of compression capabilities, which should allow to handle non-smooth problems. The potential of the method also relies on its moderate intrusive behaviour, compared to e.g. spectral Galerkin projection, where a theoretical manipulation of the original system is needed.

Several activities are planned to generalize our initial work, and to apply it to complex flows in multiple (space) dimensions and with many uncertain parameters.

The first is the improvement of the efficiency. This may be achieved by means of anisotropic mesh refinement, and by experimenting with a strong parallelization of the method. Concerning the first point, we will investigate several anisotropic refinement criteria existing in literature (also in the UQ framework), starting with those already used in the team to adapt the physical grid. Concerning the implementation, the scheme formulated in [59] is conceived to be highly parallel due to the external cycle on the number of dimensions in the space of uncertain parameters. In principle, a number of parallel threads equal to the number of spatial cells could be employed. The scheme should be developed and tested for treating unsteady and discontinuous probability density function, and correlated random variables. Both the compression capabilities and the accuracy of the scheme (in the stochastic space) should be enhanced with a high-order multidimensional conservative and non-oscillatory polynomial reconstruction (ENO/WENO).

Another main objective is related to the use of multiresolution in both physical and stochastic space. This requires a careful handling of data and an updated definition of the wavelet. Until now, only a weak coupling has been performed, since the number of points in the stochastic space varies according to the physical space, but the number of points in the physical space remains unchanged. Several works exist on the multiresolution approach for image compression, but this could be the first time i in which this kind of approach would be applied at the same time in the two spaces with an unsteady procedure for refinement (and coarsening). The experimental code developed using these technologies will have to fully exploit the processing capabilities of modern massively parallel architectures, since there is a unique mesh to handle in the coupled physical/stochastic space.

3.4. Robust multi-fidelity modelling for optimization and certification

Due to the computational cost, it is of prominent importance to consider multi-fidelity approaches gathering high-fidelity and low-fidelity computations. Note that low-fidelity solutions can be given by both the use of surrogate models in the stochastic space, and/or eventually some simplified choices of physical models of some element of the system. Procedures which deal with optimization considering uncertainties for complex problems may require the evaluation of costly objective and constraint functions hundreds or even thousands of times. The associated costs are usually prohibitive. For these reason, the robustness of the optimal solution should be assessed, thus requiring the formulation of efficient methods for coupling optimization and stochastic spaces. Different approaches will be explored. Work will be developed along three axes:

1. a robust strategy using the statistics evaluation will be applied separately, *i.e.* using only low or high-fidelity evaluations. Some classical optimization algorithms will be used in this case. Influence of high-order statistics and model reduction in the robust design optimization will be explored, also by further developing some low-cost methods for robust design optimization working on the so-called Simplex^2 method [82] ;
2. a multi-fidelity strategy by using in an efficient way low fidelity and high-fidelity estimators both in physical and stochastic space will be conceived, by using a Bayesian framework for taking into account model discrepancy and a PC expansion model for building a surrogate model ;
3. develop advanced methods for robust optimization. In particular, the Simplex^2 method will be modified for introducing a hierarchical refinement with the aim to reduce the number of stochastic samples according to a given design in an adaptive way.

This work is related to the activities foreseen in the EU contract MIDWEST, in the ANR LabCom project VIPER (currently under evaluation), in a joint project with DGA and VKI, in two projects under way with AIRBUS and SAFRAN-HERAKLES.

COMMANDS Project-Team

3. Research Program

3.1. Historical aspects

The roots of deterministic optimal control are the “classical” theory of the calculus of variations, illustrated by the work of Newton, Bernoulli, Euler, and Lagrange (whose famous multipliers were introduced in [45]), with improvements due to the “Chicago school”, Bliss [32] during the first part of the 20th century, and by the notion of relaxed problem and generalized solution (Young [51]).

Trajectory optimization really started with the spectacular achievement done by Pontryagin’s group [50] during the fifties, by stating, for general optimal control problems, nonlocal optimality conditions generalizing those of Weierstrass. This motivated the application to many industrial problems (see the classical books by Bryson and Ho [38], Leitmann [47], Lee and Markus [46], Ioffe and Tihomirov [43]).

Dynamic programming was introduced and systematically studied by R. Bellman during the fifties. The HJB equation, whose solution is the value function of the (parameterized) optimal control problem, is a variant of the classical Hamilton-Jacobi equation of mechanics for the case of dynamics parameterized by a control variable. It may be viewed as a differential form of the dynamic programming principle. This nonlinear first-order PDE appears to be well-posed in the framework of *viscosity solutions* introduced by Crandall and Lions [39]. The theoretical contributions in this direction did not cease growing, see the books by Barles [30] and Bardi and Capuzzo-Dolcetta [29].

3.2. Trajectory optimization

The so-called *direct methods* consist in an optimization of the trajectory, after having discretized time, by a nonlinear programming solver that possibly takes into account the dynamic structure. So the two main problems are the choice of the discretization and the nonlinear programming algorithm. A third problem is the possibility of refinement of the discretization once after solving on a coarser grid.

In the *full discretization approach*, general Runge-Kutta schemes with different values of control for each inner step are used. This allows to obtain and control high orders of precision, see Hager [42], Bonnans [35]. In an interior-point algorithm context, controls can be eliminated and the resulting system of equation is easily solved due to its band structure. Discretization errors due to constraints are discussed in Dontchev et al. [40]. See also Malanowski et al. [48].

In the *indirect* approach, the control is eliminated thanks to Pontryagin’s maximum principle. One has then to solve the two-points boundary value problem (with differential variables state and costate) by a single or multiple shooting method. The questions are here the choice of a discretization scheme for the integration of the boundary value problem, of a (possibly globalized) Newton type algorithm for solving the resulting finite dimensional problem in IR^n (n is the number of state variables), and a methodology for finding an initial point.

For state constrained problems or singular arcs, the formulation of the shooting function may be quite elaborate [33], [34], [28]. As initiated in [41], we focus more specifically on the handling of discontinuities, with ongoing work on the geometric integration aspects (Hamiltonian conservation).

3.3. Hamilton-Jacobi-Bellman approach

This approach consists in calculating the value function associated with the optimal control problem, and then synthesizing the feedback control and the optimal trajectory using Pontryagin’s principle. The method has the great particular advantage of reaching directly the global optimum, which can be very interesting when the problem is not convex.

Characterization of the value function >From the dynamic programming principle, we derive a characterization of the value function as being a solution (in viscosity sense) of an Hamilton-Jacobi-Bellman equation, which is a nonlinear PDE of dimension equal to the number n of state variables. Since the pioneer works of Crandall and Lions [39], many theoretical contributions were carried out, allowing an understanding of the properties of the value function as well as of the set of admissible trajectories. However, there remains an important effort to provide for the development of effective and adapted numerical tools, mainly because of numerical complexity (complexity is exponential with respect to n).

Optimal stochastic control problems occur when the dynamical system is uncertain. A decision typically has to be taken at each time, while realizations of future events are unknown (but some information is given on their distribution of probabilities). In particular, problems of economic nature deal with large uncertainties (on prices, production and demand). Specific examples are the portfolio selection problems in a market with risky and non-risky assets, super-replication with uncertain volatility, management of power resources (dams, gas). Air traffic control is another example of such problems.

Nonsmoothness of the value function. Sometimes the value function is smooth and the associated HJB equation can be solved explicitly. Still, the value function is not smooth enough to satisfy the HJB equation in the classical sense. As for the deterministic case, the notion of viscosity solution provides a convenient framework for dealing with the lack of smoothness, see Pham [49], that happens also to be well adapted to the study of discretization errors for numerical discretization schemes [44], [31].

For solving stochastic control problems, we studied the so-called Generalized Finite Differences (GFD), that allow to choose at any node, the stencil approximating the diffusion matrix up to a certain threshold [37]. Determining the stencil and the associated coefficients boils down to a quadratic program to be solved at each point of the grid, and for each control. This is definitely expensive, with the exception of special structures where the coefficients can be computed at low cost. For two dimensional systems, we designed a (very) fast algorithm for computing the coefficients of the GFD scheme, based on the Stern-Brocot tree [36].

CQFD Project-Team

3. Research Program

3.1. Introduction

The scientific objectives of the team are to provide mathematical tools for modeling and optimization of complex systems. These systems require mathematical representations which are in essence dynamic, multi-model and stochastic. This increasing complexity poses genuine scientific challenges in the domain of modeling and optimization. More precisely, our research activities are focused on stochastic optimization and (parametric, semi-parametric, multidimensional) statistics which are complementary and interlinked topics. It is essential to develop simultaneously statistical methods for the estimation and control methods for the optimization of the models.

3.2. Main research topics

- Stochastic modeling: Markov chain, Piecewise Deterministic Markov Processes (PDMP), Markov Decision Processes (MDP).
  The mathematical representation of complex systems is a preliminary step to our final goal corresponding to the optimization of its performance. For example, in order to optimize the predictive maintenance of a system, it is necessary to choose the adequate model for its representation. The step of modeling is crucial before any estimation or computation of quantities related to its optimization. For this we have to represent all the different regimes of the system and the behavior of the physical variables under each of these regimes. Moreover, we must also select the dynamic variables which have a potential effect on the physical variable and the quantities of interest. The team CQFD works on the theory of Piecewise Deterministic Markov Processes (PDMP's) and on Markov Decision Processes (MDP's). These two classes of systems form general families of controlled stochastic processes suitable for the modeling of sequential decision-making problems in the continuous-time (PDMPs) and discrete-time (MDP's) context. They appear in many fields such as engineering, computer science, economics, operations research and constitute powerful class of processes for the modeling of complex system.
- Estimation methods: estimation for PDMP; estimation in non- and semi parametric regression modeling.
  To the best of our knowledge, there does not exist any general theory for the problems of estimating parameters of PDMPs although there already exist a large number of tools for sub-classes of PDMPs such as point processes and marked point processes. However, to fill the gap between these specific models and the general class of PDMPs, new theoretical and mathematical developments will be on the agenda of the whole team. In the framework of non-parametric regression or quantile regression, we focus on kernel estimators or kernel local linear estimators for complete data or censored data. New strategies for estimating semi-parametric models via recursive estimation procedures have also received an increasing interest recently. The advantage of the recursive estimation approach is to take into account the successive arrivals of the information and to refine, step after step, the implemented estimation algorithms. These recursive methods do require restarting calculation of parameter estimation from scratch when new data are added to the base. The idea is to use only the previous estimations and the new data to refresh the estimation. The gain in time could be very interesting and there are many applications of such approaches.

- Dimension reduction: dimension-reduction via SIR and related methods, dimension-reduction via multidimensional and classification methods.
  Most of the dimension reduction approaches seek for lower dimensional subspaces minimizing the loss of some statistical information. This can be achieved in modeling framework or in exploratory data analysis context.
  In modeling framework we focus our attention on semi-parametric models in order to conjugate the advantages of parametric and nonparametric modeling. On the one hand, the parametric part of the model allows a suitable interpretation for the user. On the other hand, the functional part of the model offers a lot of flexibility. In this project, we are especially interested in the semi-parametric regression model $Y = f(X'\theta) + \varepsilon$, the unknown parameter θ belongs to $\mathbb{R}^p$ for a single index model, or is such that $\theta = [\theta_1, \cdots, \theta_d]$ (where each θ_k belongs to $\mathbb{R}^p$ and $d \leq p$ for a multiple indices model), the noise ε is a random error with unknown distribution, and the link function f is an unknown real valued function. Another way to see this model is the following: the variables X and Y are independent given $X'\theta$. In our semi-parametric framework, the main objectives are to estimate the parametric part θ as well as the nonparametric part which can be the link function f, the conditional distribution function of Y given X or the conditional quantile q_α. In order to estimate the dimension reduction parameter θ we focus on the Sliced Inverse Regression (SIR) method which has been introduced by Li [44] and Duan and Li [42].
  Methods of dimension reduction are also important tools in the field of data analysis, data mining and machine learning.They provide a way to understand and visualize the structure of complex data sets.Traditional methods among others are principal component analysis for quantitative variables or multiple component analysis for qualitative variables. New techniques have also been proposed to address these challenging tasks involving many irrelevant and redundant variables and often comparably few observation units. In this context, we focus on the problem of synthetic variables construction, whose goals include increasing the predictor performance and building more compact variables subsets. Clustering of variables is used for feature construction. The idea is to replace a group of ”similar” variables by a cluster centroid, which becomes a feature. The most popular algorithms include K-means and hierarchical clustering. For a review, see, e.g., the textbook of Duda [43].
- Stochastic optimal control: optimal stopping, impulse control, continuous control, linear programming.
  The first objective is to focus on the development of computational methods.
  - In the continuous-time context, stochastic control theory has from the numerical point of view, been mainly concerned with Stochastic Differential Equations (SDEs in short). From the practical and theoretical point of view, the numerical developments for this class of processes are extensive and largely complete. It capitalizes on the connection between SDEs and second order partial differential equations (PDEs in short) and the fact that the properties of the latter equations are very well understood. It is, however, hard to deny that the development of computational methods for the control of PDMPs has received little attention. One of the main reasons is that the role played by the familiar PDEs in the diffusion models is here played by certain systems of integro-differential equations for which there is not (and cannot be) a unified theory such as for PDEs as emphasized by M.H.A. Davis in his book. To the best knowledge of the team, there is only one attempt to tackle this difficult problem by O.L.V. Costa and M.H.A. Davis. The originality of our project consists in studying this unexplored area. It is very important to stress the fact that these numerical developments will give rise to a lot of theoretical issues such as type of approximations, convergence results, rates of convergence,....
  - Theory for MDP’s has reached a rather high degree of maturity, although the classical tools such as value iteration, policy iteration and linear programming, and their various extensions, are not applicable in practice. We believe that the theoretical progress of MDP’s must be in parallel with the corresponding numerical developments. Therefore, solving

MDP’s numerically is an awkward and important problem both from the theoretical and practical point of view. In order to meet this challenge, the fields of neural networks, neuro-dynamic programming and approximate dynamic programming became recently an active area of research. Such methods found their roots in heuristic approaches, but theoretical results for convergence results are mainly obtained in the context of finite MDP’s. Hence, an ambitious challenge is to investigate such numerical problems but for models with general state and action spaces. Our motivation is to develop theoretically consistent computational approaches for approximating optimal value functions and finding optimal policies.

– An effort has been devoted to the development of efficient computational methods in the setting of communication networks. These are complex dynamical systems composed of several interacting nodes that exhibit important congestion phenomena as their level of interaction grows. The dynamics of such systems are affected by the randomness of their underlying events (e.g., arrivals of http requests to a web-server) and are described stochastically in terms of queueing network models. These are mathematical tools that allow one to predict the performance achievable by the system, to optimize the network configuration, to perform capacity-planning studies, etc. These objectives are usually difficult to achieve without a mathematical model because Internet systems are huge in size. However, because of the exponential growth of their state spaces, an exact analysis of queueing network models is generally difficult to obtain. Given this complexity, we have developed analyses in some limiting regime of practical interest (e.g., systems size grows to infinity). This approach is helpful to obtain a simpler mathematical description of the system under investigation, which leads to the direct definition of efficient, though approximate, computational methods and also allows to investigate other aspects such as Nash equilibria.

The second objective of the team is to study some theoretical aspects related to MDPs such as convex analytical methods and singular perturbation. Analysis of various problems arising in MDPs leads to a large variety of interesting mathematical problems.

DEFI Project-Team

3. Research Program

3.1. Research Program

The research activity of our team is dedicated to the design, analysis and implementation of efficient numerical methods to solve inverse and shape/topological optimization problems in connection with wave imaging, structural design, non-destructive testing and medical imaging modalities. We are particularly interested in the development of fast methods that are suited for real-time applications and/or large scale problems. These goals require to work on both the physical and the mathematical models involved and indeed a solid expertise in related numerical algorithms.

This section intends to give a general overview of our research interests and themes. We choose to present them through the specific academic example of inverse scattering problems (from inhomogeneities), which is representative of foreseen developments on both inversion and (topological) optimization methods. The practical problem would be to identify an inclusion from measurements of diffracted waves that result from the interaction of the sought inclusion with some (incident) waves sent into the probed medium. Typical applications include biomedical imaging where using micro-waves one would like to probe the presence of pathological cells, or imaging of urban infrastructures where using ground penetrating radars (GPR) one is interested in finding the location of buried facilities such as pipelines or waste deposits. This kind of applications requires in particular fast and reliable algorithms.

By “imaging” we shall refer to the inverse problem where the concern is only the location and the shape of the inclusion, while “identification” may also indicate getting informations on the inclusion physical parameters.

Both problems (imaging and identification) are non linear and ill-posed (lack of stability with respect to measurements errors if some careful constrains are not added). Moreover, the unique determination of the geometry or the coefficients is not guaranteed in general if sufficient measurements are not available. As an example, in the case of anisotropic inclusions, one can show that an appropriate set of data uniquely determine the geometry but not the material properties.

These theoretical considerations (uniqueness, stability) are not only important in understanding the mathematical properties of the inverse problem, but also guide the choice of appropriate numerical strategies (which information can be stably reconstructed) and also the design of appropriate regularization techniques. Moreover, uniqueness proofs are in general constructive proofs, i.e. they implicitly contain a numerical algorithm to solve the inverse problem, hence their importance for practical applications. The sampling methods introduced below are one example of such algorithms.

A large part of our research activity is dedicated to numerical methods applied to the first type of inverse problems, where only the geometrical information is sought. In its general setting the inverse problem is very challenging and no method can provide a universal satisfactory solution to it (regarding the balance cost-precision-stability). This is why in the majority of the practically employed algorithms, some simplification of the underlying mathematical model is used, according to the specific configuration of the imaging experiment. The most popular ones are geometric optics (the Kirchhoff approximation) for high frequencies and weak scattering (the Born approximation) for small contrasts or small obstacles. They actually give full satisfaction for a wide range of applications as attested by the large success of existing imaging devices (radar, sonar, ultrasound, X-ray tomography, etc.), that rely on one of these approximations.

Generally speaking, the used simplifications result in a linearization of the inverse problem and therefore are usually valid only if the latter is weakly non-linear. The development of these simplified models and the improvement of their efficiency is still a very active research area. With that perspective we are particularly interested in deriving and studying higher order asymptotic models associated with small geometrical parameters such as: small obstacles, thin coatings, wires, periodic media, ... Higher order models usually introduce some non linearity in the inverse problem, but are in principle easier to handle from the numerical point of view than in the case of the exact model.

A larger part of our research activity is dedicated to algorithms that avoid the use of such approximations and that are efficient where classical approaches fail: i.e. roughly speaking when the non linearity of the inverse problem is sufficiently strong. This type of configuration is motivated by the applications mentioned below, and occurs as soon as the geometry of the unknown media generates non negligible multiple scattering effects (multiply-connected and closely spaces obstacles) or when the used frequency is in the so-called resonant region (wave-length comparable to the size of the sought medium). It is therefore much more difficult to deal with and requires new approaches. Our ideas to tackle this problem will be motivated and inspired by recent advances in shape and topological optimization methods and also the introduction of novel classes of imaging algorithms, so-called sampling methods.

The sampling methods are fast imaging solvers adapted to multi-static data (multiple receiver-transmitter pairs) at a fixed frequency. Even if they do not use any linearization the forward model, they rely on computing the solutions to a set of linear problems of small size, that can be performed in a completely parallel procedure. Our team has already a solid expertise in these methods applied to electromagnetic 3-D problems. The success of such approaches was their ability to provide a relatively quick algorithm for solving 3-D problems without any need for a priori knowledge on the physical parameters of the targets. These algorithms solve only the imaging problem, in the sense that only the geometrical information is provided.

Despite the large efforts already spent in the development of this type of methods, either from the algorithmic point of view or the theoretical one, numerous questions are still open. These attractive new algorithms also suffer from the lack of experimental validations, due to their relatively recent introduction. We also would like to invest on this side by developing collaborations with engineering research groups that have experimental facilities. From the practical point of view, the most potential limitation of sampling methods would be the need of a large amount of data to achieve a reasonable accuracy. On the other hand, optimization methods do not suffer from this constrain but they require good initial guess to ensure convergence and reduce the number of iterations. Therefore it seems natural to try to combine the two class of methods in order to calibrate the balance between cost and precision.

Among various shape optimization methods, the Level Set method seems to be particularly suited for such a coupling. First, because it shares similar mechanism as sampling methods: the geometry is captured as a level set of an “indicator function” computed on a cartesian grid. Second, because the two methods do not require any a priori knowledge on the topology of the sought geometry. Beyond the choice of a particular method, the main question would be to define in which way the coupling can be achieved. Obvious strategies consist in using one method to pre-process (initialization) or post-process (find the level set) the other. But one can also think of more elaborate ones, where for instance a sampling method can be used to optimize the choice of the incident wave at each iteration step.The latter point is closely related to the design of so called “focusing incident waves” (which are for instance the basis of applications of the time-reversal principle). In the frequency regime, these incident waves can be constructed from the eigenvalue decomposition of the data operator used by sampling methods. The theoretical and numerical investigations of these aspects are still not completely understood for electromagnetic or elastodynamic problems.

Other topological optimization methods, like the homogenization method or the topological gradient method, can also be used, each one provides particular advantages in specific configurations. It is evident that the development of these methods is very suited to inverse problems and provide substantial advantage compared to classical shape optimization methods based on boundary variation. Their applications to inverse problems has not been fully investigated. The efficiency of these optimization methods can also be increased for adequate asymptotic configurations. For instance small amplitude homogenization method can be used as an efficient relaxation method for the inverse problem in the presence of small contrasts. On the other hand, the topological gradient method has shown to perform well in localizing small inclusions with only one iteration.

A broader perspective would be the extension of the above mentioned techniques to time-dependent cases. Taking into account data in time domain is important for many practical applications, such as imaging in cluttered media, the design of absorbing coatings or also crash worthiness in the case of structural design.

For the identification problem, one would like to also have information on the physical properties of the targets. Of course optimization methods is a tool of choice for these problems. However, in some applications only a qualitative information is needed and obtaining it in a cheaper way can be performed using asymptotic theories combined with sampling methods. We also refer here to the use of so called transmission eigenvalues as qualitative indicators for non destructive testing of dielectrics.

We are also interested in parameter identification problems arising in diffusion-type problems. Our research here is mostly motivated by applications to the imaging of biological tissues with the technique of Diffusion Magnetic Resonance Imaging (DMRI). Roughly speaking DMRI gives a measure of the average distance travelled by water molecules in a certain medium and can give useful information on cellular structure and structural change when the medium is biological tissue. In particular, we would like to infer from DMRI measurements changes in the cellular volume fraction occurring upon various physiological or pathological conditions as well as the average cell size in the case of tumor imaging. The main challenges here are 1) correctly model measured signals using diffusive-type time-dependent PDEs 2) numerically handle the complexity of the tissues 3) use the first two to identify physically relevant parameters from measurements. For the last point we are particularly interested in constructing reduced models of the multiple-compartment Bloch-Torrey partial differential equation using homogenization methods.

DISCO Project-Team

3. Research Program

3.1. Modeling of complex environment

We want to model phenomena such as a temporary loss of connection (e.g. synchronisation of the movements through haptic interfaces), a nonhomogeneous environment (e.g. case of cryogenic systems) or the presence of the human factor in the control loop (e.g. grid systems) but also problems involved with technological constraints (e.g. range of the sensors). The mathematical models concerned include integro-differential, partial differential equations, algebraic inequalities with the presence of several time scales, whose variables and/or parameters must satisfy certain constraints (for instance, positivity).

3.2. Analysis of interconnected systems

- Robust stability of linear systems

  Within an interconnection context, lots of phenomena are modelled directly or after an approximation by delay systems. These systems might have fixed delays, time-varying delays, distributed delays ...

  For various infinite-dimensional systems, particularly delay and fractional systems, input-output and time-domain methods are jointly developed in the team to characterize stability. This research is developed at four levels: analytic approaches (H_∞-stability, BIBO-stablity, robust stability, robustness metrics) [1], [2], [5], [6], symbolic computation approaches (SOS methods are used for determining easy-to-check conditions which guarantee that the poles of a given linear system are not in the closed right half-plane, certified CAD techniques), numerical approaches (root-loci, continuation methods) and by means of softwares developed in the team [5], [6].

- Robustness/fragility of biological systems

  Deterministic biological models describing, for instance, species interactions, are frequently composed of equations with important disturbances and poorly known parameters. To evaluate the impact of the uncertainties, we use the techniques of designing of global strict Lyapunov functions or functional developed in the team.

  However, for other biological systems, the notion of robustness may be different and this question is still in its infancy (see, e.g. [66]). Unlike engineering problems where a major issue is to maintain stability in the presence of disturbances, a main issue here is to maintain the system response in the presence of disturbances. For instance, a biological network is required to keep its functioning in case of a failure of one of the nodes in the network. The team, which has a strong expertise in robustness for engineering problems, aims at contributing at the develpment of new robustness metrics in this biological context.

3.3. Stabilization of interconnected systems

- Linear systems: Analytic and algebraic approaches are considered for infinite-dimensional linear systems studied within the input-output framework.

  In the recent years, the Youla-Kučera parametrization (which gives the set of all stabilizing controllers of a system in terms of its coprime factorizations) has been the cornerstone of the success of the H_∞-control since this parametrization allows one to rewrite the problem of finding the optimal stabilizing controllers for a certain norm such as H_∞ or H_2 as affine, and thus, convex problem.

  A central issue studied in the team is the computation of such factorizations for a given infinite-dimensional linear system as well as establishing the links between stabilizability of a system for a certain norm and the existence of coprime factorizations for this system. These questions are fundamental for robust stabilization problems [1], [2].

We also consider simultaneous stabilization since it plays an important role in the study of reliable stabilization, i.e. in the design of controllers which stabilize a finite family of plants describing a system during normal operating conditions and various failed modes (e.g. loss of sensors or actuators, changes in operating points). Moreover, we investigate strongly stabilizable systems, namely systems which can be stabilized by stable controllers, since they have a good ability to track reference inputs and, in practice, engineers are reluctant to use unstable controllers especially when the system is stable.

- Nonlinear systems

  The project aims at developing robust stabilization theory and methods for important classes of nonlinear systems that ensure good controllerperformance under uncertainty and time delays. The main techniques include techniques called backstepping and forwarding, contructions of strict Lyapunov functions through so-called "strictification" approaches [3] and construction of Lyapunov-Krasovskii functionals [4], [5], [6].

- Predictive control

  For highly complex systems described in the time-domain and which are submitted to constraints, predictive control seems to be well-adapted. This model based control method (MPC: Model Predictive Control) is founded on the determination of an optimal control sequence over a receding horizon. Due to its formulation in the time-domain, it is an effective tool for handling constraints and uncertainties which can be explicitly taken into account in the synthesis procedure [7]. The team considers how mutiparametric optimization can help to reduce the computational load of this method, allowing its effective use on real world constrained problems.

  The team also investigates stochastic optimization methods such as genetic algorithm, particle swarm optimization or ant colony [8] as they can be used to optimize any criterion and constraint whatever their mathematical structure is. The developed methodologies can be used by non specialists.

3.4. Synthesis of reduced complexity controllers

- PID controllers

  Even though the synthesis of control laws of a given complexity is not a new problem, it is still open, even for finite-dimensional linear systems. Our purpose is to search for good families of “simple” (e.g. low order) controllers for infinite-dimensional dynamical systems. Within our approach, PID candidates are first considered in the team [2], [67].

- Predictive control

  The synthesis of predictive control laws is concerned with the solution of multiparametric optimization problems. Reduced order controller constraints can be viewed as non convex constraints in the synthesis procedure. Such constraints can be taken into account with stochastic algorithms.

Finally, the development of algorithms based on both symbolic computation and numerical methods, and their implementations in dedicated Scilab/Matlab/Maple toolboxes are important issues in the project.

DOLPHIN Project-Team

3. Research Program

3.1. Hybrid multi-objective optimization methods

The success of metaheuristics is based on their ability to find efficient solutions in a reasonable time [54]. But with very large problems and/or multi-objective problems, efficiency of metaheuristics may be compromised. Hence, in this context it is necessary to integrate metaheuristics in more general schemes in order to develop even more efficient methods. For instance, this can be done by different strategies such as cooperation and parallelization.

The DOLPHIN project deals with *"a posteriori"* multi-objective optimization where the set of Pareto solutions (solutions of best compromise) have to be generated in order to give the decision maker the opportunity to choose the solution that interests him/her.

Population-based methods, such as evolutionary algorithms, are well fitted for multi-objective problems, as they work with a set of solutions [50], [53]. To be convinced one may refer to the list of references on Evolutionary Multi-objective Optimization maintained by Carlos A. Coello [0], which contains more than 5500 references. One of the objectives of the project is to propose advanced search mechanisms for intensification and diversification. These mechanisms have been designed in an adaptive manner, since their effectiveness is related to the landscape of the MOP and to the instance solved.

In order to assess the performances of the proposed mechanisms, we always proceed in two steps: first, we carry out experiments on academic problems, for which some best known results exist; second, we use real industrial problems to cope with large and complex MOPs. The lack of references in terms of optimal or best known Pareto set is a major problem. Therefore, the obtained results in this project and the test data sets will be available at the URL http://dolphin.lille.inria.fr/ at 'benchmark'.

3.1.1. Cooperation of metaheuristics

In order to benefit from the various advantages of the different metaheuristics, an interesting idea is to combine them. Indeed, the hybridization of metaheuristics allows the cooperation of methods having complementary behaviors. The efficiency and the robustness of such methods depend on the balance between the exploration of the whole search space and the exploitation of interesting areas.

Hybrid metaheuristics have received considerable interest these last years in the field of combinatorial optimization. A wide variety of hybrid approaches have been proposed in the literature and give very good results on numerous single objective optimization problems, which are either academic (traveling salesman problem, quadratic assignment problem, scheduling problem, etc) or real-world problems. This efficiency is generally due to the combinations of single-solution based methods (iterative local search, simulated annealing, tabu search, etc) with population-based methods (genetic algorithms, ants search, scatter search, etc). A taxonomy of hybridization mechanisms may be found in [56]. It proposes to decompose these mechanisms into four classes:

- *LRH class - Low-level Relay Hybrid*: This class contains algorithms in which a given metaheuristic is embedded into a single-solution metaheuristic. Few examples from the literature belong to this class.
- *LTH class - Low-level Teamwork Hybrid*: In this class, a metaheuristic is embedded into a population-based metaheuristic in order to exploit strengths of single-solution and population-based metaheuristics.

[0] http://delta.cs.cinvestav.mx/~ccoello/EMOO/EMOObib.html

- *HRH class - High-level Relay Hybrid*: Here, self contained metaheuristics are executed in a sequence. For instance, a population-based metaheuristic is executed to locate interesting regions and then a local search is performed to exploit these regions.
- *HTH class - High-level Teamwork Hybrid*: This scheme involves several self-contained algorithms performing a search in parallel and cooperating. An example will be the island model, based on GAs, where the population is partitioned into small subpopulations and a GA is executed per subpopulation. Some individuals can migrate between subpopulations.

Let us notice that, hybrid methods have been studied in the mono-criterion case, their application in the multi-objective context is not yet widely spread. The objective of the DOLPHIN project is to integrate specificities of multi-objective optimization into the definition of hybrid models.

3.1.2. Cooperation between metaheuristics and exact methods

Until now only few exact methods have been proposed to solve multi-objective problems. They are based either on a Branch-and-bound approach, on the algorithm $A^{\star}$, or on dynamic programming. However, these methods are limited to two objectives and, most of the time, cannot be used on a complete large scale problem. Therefore, sub search spaces have to be defined in order to use exact methods. Hence, in the same manner as hybridization of metaheuristics, the cooperation of metaheuristics and exact methods is also a main issue in this project. Indeed, it allows us to use the exploration capacity of metaheuristics, as well as the intensification ability of exact methods, which are able to find optimal solutions in a restricted search space. Sub search spaces have to be defined along the search. Such strategies can be found in the literature, but they are only applied to mono-objective academic problems.

We have extended the previous taxonomy for hybrid metaheuristics to the cooperation between exact methods and metaheuristics. Using this taxonomy, we are investigating cooperative multi-objective methods. In this context, several types of cooperations may be considered, according to the way the metaheuristic and the exact method cooperate. For instance, a metaheuristic can use an exact method for intensification or an exact method can use a metaheuristic to reduce the search space.

Moreover, a part of the DOLPHIN project deals with studying exact methods in the multi-objective context in order: i) to be able to solve small size problems and to validate proposed heuristic approaches; ii) to have more efficient/dedicated exact methods that can be hybridized with metaheuristics. In this context, the use of parallelism will push back limits of exact methods, which will be able to explore larger size search spaces [51].

3.1.3. Goals

Based on the previous works on multi-objective optimization, it appears that to improve metaheuristics, it becomes essential to integrate knowledge about the problem structure. This knowledge can be gained during the search. This would allow us to adapt operators which may be specific for multi-objective optimization or not. The goal here is to design auto-adaptive methods that are able to react to the problem structure. Moreover, regarding the hybridization and the cooperation aspects, the objectives of the DOLPHIN project are to deepen these studies as follows:

- *Design of metaheuristics for the multi-objective optimization:* To improve metaheuristics, it becomes essential to integrate knowledge about the problem structure, which we may get during the execution. This would allow us to adapt operators that may be specific for multi-objective optimization or not. The goal here is to design auto-adaptive methods that are able to react to the problem structure.
- *Design of cooperative metaheuristics:* Previous studies show the interest of hybridization for a global optimization and the importance of problem structure study for the design of efficient methods. It is now necessary to generalize hybridization of metaheuristics and to propose adaptive hybrid models that may evolve during the search while selecting the appropriate metaheuristic. Multi-objective aspects have to be introduced in order to cope with the specificities of multi-objective optimization.

- *Design of cooperative schemes between exact methods and metaheuristics:* Once the study on possible cooperation schemes is achieved, we will have to test and compare them in the multi-objective context.
- *Design and conception of parallel metaheuristics:* Our previous works on parallel metaheuristics allow us to speed up the resolution of large scale problems. It could be also interesting to study the robustness of the different parallel models (in particular in the multi-objective case) and to propose rules that determine, given a specific problem, which kind of parallelism to use. Of course these goals are not disjoined and it will be interesting to simultaneously use hybrid metaheuristics and exact methods. Moreover, those advanced mechanisms may require the use of parallel and distributed computing in order to easily make cooperating methods evolve simultaneously and to speed up the resolution of large scale problems.
- *Validation:* In order to validate the obtained results we always proceed in two phases: validation on academic problems, for which some best known results exist and use on real problems (industrial) to cope with problem size constraints.

  Moreover, those advanced mechanisms are to be used in order to integrate the distributed multi-objective aspects in the ParadisEO platform (see the paragraph on software platform).

3.2. Parallel multi-objective optimization: models and software frameworks

Parallel and distributed computing may be considered as a tool to speedup the search to solve large MOPs and to improve the robustness of a given method. Moreover, the joint use of parallelism and cooperation allows improvements on the quality of the obtained Pareto sets. Following this objective, we will design and implement parallel models for metaheuristics (evolutionary algorithms, tabu search approach) and exact methods (branch-and-bound algorithm, branch-and-cut algorithm) to solve different large MOPs.

One of the goals of the DOLPHIN project is to integrate the developed parallel models into software frameworks. Several frameworks for parallel distributed metaheuristics have been proposed in the literature. Most of them focus only either on evolutionary algorithms or on local search methods. Only few frameworks are dedicated to the design of both families of methods. On the other hand, existing optimization frameworks either do not provide parallelism at all or just supply at most one parallel model. In this project, a new framework for parallel hybrid metaheuristics is proposed, named *Parallel and Distributed Evolving Objects (ParadisEO)* based on EO. The framework provides in a transparent way the hybridization mechanisms presented in the previous section, and the parallel models described in the next section. Concerning the developed parallel exact methods for MOPs, we will integrate them into well-known frameworks such as COIN.

3.2.1. Parallel models

According to the family of addressed metaheuristics, we may distinguish two categories of parallel models: parallel models that manage a single solution, and parallel models that handle a population of solutions. The major single solution-based parallel models are the following: the *parallel neighborhood exploration model* and the *multi-start model.*

- *The parallel neighborhood exploration model* is basically a "low level" model that splits the neighborhood into partitions that are explored and evaluated in parallel. This model is particularly interesting when the evaluation of each solution is costly and/or when the size of the neighborhood is large. It has been successfully applied to the mobile network design problem (see Application section).
- *The multi-start model* consists in executing in parallel several local searches (that may be heterogeneous), without any information exchange. This model raises particularly the following question: is it equivalent to execute k local searches during a time t than executing a single local search during $k \times t$? To answer this question we tested a multi-start Tabu search on the quadratic assignment problem. The experiments have shown that the answer is often landscape-dependent. For example, the multi-start model may be well-suited for landscapes with multiple basins.

Parallel models that handle a population of solutions are mainly: the *island model*, the *central model* and *the distributed evaluation of a single solution*. Let us notice that the last model may also be used with single-solution metaheuristics.

- In *the island model*, the population is split into several sub-populations distributed among different processors. Each processor is responsible of the evolution of one sub-population. It executes all the steps of the metaheuristic from the selection to the replacement. After a given number of generations (synchronous communication), or when a convergence threshold is reached (asynchronous communication), the migration process is activated. Then, exchanges of solutions between sub-populations are realized, and received solutions are integrated into the local sub-population.
- *The central (Master/Worker) model* allows us to keep the sequentiality of the original algorithm. The master centralizes the population and manages the selection and the replacement steps. It sends sub-populations to the workers that execute the recombination and evaluation steps. The latter returns back newly evaluated solutions to the master. This approach is efficient when the generation and evaluation of new solutions is costly.
- *The distributed evaluation model* consists in a parallel evaluation of each solution. This model has to be used when, for example, the evaluation of a solution requires access to very large databases (data mining applications) that may be distributed over several processors. It may also be useful in a multi-objective context, where several objectives have to be computed simultaneously for a single solution.

As these models have now been identified, our objective is to study them in the multi-objective context in order to use them advisedly. Moreover, these models may be merged to combine different levels of parallelism and to obtain more efficient methods [52], [55].

3.2.2. Goals

Our objectives focus on these issues are the following:

- *Design of parallel models for metaheuristics and exact methods for MOPs*: We will develop parallel cooperative metaheuristics (evolutionary algorithms and local search algorithms such as the Tabu search) for solving different large MOPs. Moreover, we are designing a new exact method, named PPM (Parallel Partition Method), based on branch and bound and branch and cut algorithms. Finally, some parallel cooperation schemes between metaheuristics and exact algorithms have to be used to solve MOPs in an efficient manner.
- *Integration of the parallel models into software frameworks*: The parallel models for metaheuristics will be integrated in the ParadisEO software framework. The proposed multi-objective exact methods must be first integrated into standard frameworks for exact methods such as COIN and BOB++. A *coupling* with ParadisEO is then needed to provide hybridization between metaheuristics and exact methods.
- *Efficient deployment of the parallel models on different parallel and distributed architectures including GRIDs*: The designed algorithms and frameworks will be efficiently deployed on non-dedicated networks of workstations, dedicated cluster of workstations and SMP (Symmetric Multi-processors) machines. For GRID computing platforms, peer to peer (P2P) middlewares (XtremWeb-Condor) will be used to implement our frameworks. For this purpose, the different optimization algorithms may be re-visited for their efficient deployment.

ECUADOR Project-Team

3. Research Program

3.1. Algorithmic Differentiation

Participants: Laurent Hascoët, Valérie Pascual, Ala Taftaf.

algorithmic differentiation (AD, aka Automatic Differentiation) Transformation of a program, that returns a new program that computes derivatives of the initial program, i.e. some combination of the partial derivatives of the program's outputs with respect to its inputs.

adjoint Mathematical manipulation of the Partial Differential Equations that define a problem, obtaining new differential equations that define the gradient of the original problem's solution.

checkpointing General trade-off technique, used in adjoint AD, that trades duplicate execution of a part of the program to save some memory space that was used to save intermediate results.

Algorithmic Differentiation (AD) differentiates *programs*. The input of AD is a source program P that, given some $X \in \mathbb{R}^n$, returns some $Y = F(X) \in \mathbb{R}^m$, for a differentiable F. AD generates a new source program P' that, given X, computes some derivatives of F [6].

Any execution of P amounts to a sequence of instructions, which is identified with a composition of vector functions. Thus, if

$$\begin{array}{ccc} P & \text{runs} & \{I_1; I_2; \cdots I_p;\}, \\ F & \text{then is} & f_p \circ f_{p-1} \circ \cdots \circ f_1, \end{array} \tag{3}$$

where each f_k is the elementary function implemented by instruction I_k. AD applies the chain rule to obtain derivatives of F. Calling X_k the values of all variables after instruction I_k, i.e. $X_0 = X$ and $X_k = f_k(X_{k-1})$, the Jacobian of F is

$$F'(X) = f'_p(X_{p-1}) \,.\, f'_{p-1}(X_{p-2}) \,.\, \cdots \,.\, f'_1(X_0) \tag{4}$$

which can be mechanically written as a sequence of instructions I'_k. This can be generalized to higher level derivatives, Taylor series, etc. Combining the I'_k with the control of P yields P', and therefore this differentiation is piecewise.

In practice, many applications only need cheaper projections of $F'(X)$ such as:

- **Sensitivities**, defined for a given direction $\dot{X}$ in the input space as:

  $$F'(X).\dot{X} = f'_p(X_{p-1}) \,.\, f'_{p-1}(X_{p-2}) \,.\, \cdots \,.\, f'_1(X_0) \,.\, \dot{X} \quad . \tag{5}$$

  This expression is easily computed from right to left, interleaved with the original program instructions. This is the *tangent mode* of AD.

- **Adjoints**, defined after transposition (F'^*), for a given weighting $\overline{Y}$ of the outputs as:

  $$F'^*(X).\overline{Y} = f'^*_1(X_0).f'^*_2(X_1). \cdots .f'^*_{p-1}(X_{p-2}).f'^*_p(X_{p-1}).\overline{Y} \quad . \tag{6}$$

> This expression is most efficiently computed from right to left, because matrix×vector products are cheaper than matrix×matrix products. This is the *adjoint mode* of AD, most effective for optimization, data assimilation [37], adjoint problems [32], or inverse problems.

Adjoint AD builds a very efficient program [34], which computes the gradient in a time independent from the number of parameters n. In contrast, computing the same gradient with the *tangent mode* would require running the tangent differentiated program n times.

However, the X_k are required in the *inverse* of their computation order. If the original program *overwrites* a part of X_k, the differentiated program must restore X_k before it is used by $f'^*_{k+1}(X_k)$. Therefore, the central research problem of adjoint AD is to make the X_k available in reverse order at the cheapest cost, using strategies that combine storage, repeated forward computation from available previous values, or even inverted computation from available later values.

Another research issue is to make the AD model cope with the constant evolution of modern language constructs. From the old days of Fortran77, novelties include pointers and dynamic allocation, modularity, structured data types, objects, vectorial notation and parallel programming. We keep developing our models and tools to handle these new constructs.

3.2. Static Analysis and Transformation of programs

Participants: Laurent Hascoët, Valérie Pascual, Ala Taftaf.

abstract syntax tree Tree representation of a computer program, that keeps only the semantically significant information and abstracts away syntactic sugar such as indentation, parentheses, or separators.

control flow graph Representation of a procedure body as a directed graph, whose nodes, known as basic blocks, each contain a sequence of instructions and whose arrows represent all possible control jumps that can occur at run-time.

abstract interpretation Model that describes program static analysis as a special sort of execution, in which all branches of control switches are taken concurrently, and where computed values are replaced by abstract values from a given *semantic domain*. Each particular analysis gives birth to a specific semantic domain.

data flow analysis Program analysis that studies how a given property of variables evolves with execution of the program. Data Flow analysis is static, therefore studying all possible run-time behaviors and making conservative approximations. A typical data-flow analysis is to detect, at any location in the source program, whether a variable is initialized or not.

The most obvious example of a program transformation tool is certainly a compiler. Other examples are program translators, that go from one language or formalism to another, or optimizers, that transform a program to make it run better. AD is just one such transformation. These tools share the technological basis that lets them implement the sophisticated analyses [25] required. In particular there are common mathematical models to specify these analyses and analyze their properties.

An important principle is *abstraction*: the core of a compiler should not bother about syntactic details of the compiled program. The optimization and code generation phases must be independent from the particular input programming language. This is generally achieved using language-specific *front-ends*, language-independent *middle-ends*, and target-specific *back-ends*. In the middle-end, analysis can concentrate on the semantics of a reduced set of constructs. This analysis operates on an abstract representation of programs made of one *call graph*, whose nodes are themselves *flow graphs* whose nodes (*basic blocks*) contain abstract *syntax trees* for the individual atomic instructions. To each level are attached symbol tables, nested to capture scoping.

Static program analysis can be defined on this internal representation, which is largely language independent. The simplest analyses on trees can be specified with inference rules [28], [35], [26]. But many *data-flow analyses* are more complex, and better defined on graphs than on trees. Since both call graphs and flow graphs may be cyclic, these global analyses will be solved iteratively. *Abstract Interpretation* [29] is a theoretical framework to study complexity and termination of these analyses.

Data flow analyses must be carefully designed to avoid or control combinatorial explosion. At the call graph level, they can run bottom-up or top-down, and they yield more accurate results when they take into account the different call sites of each procedure, which is called *context sensitivity*. At the flow graph level, they can run forwards or backwards, and yield more accurate results when they take into account only the possible execution flows resulting from possible control, which is called *flow sensitivity*.

Even then, data flow analyses are limited, because they are static and thus have very little knowledge of actual run-time values. Far before reaching the very theoretical limit of *undecidability*, one reaches practical limitations to how much information one can infer from programs that use arrays [41], [30] or pointers. Therefore, conservative *over-approximations* must be made, leading to derivative code less efficient than ideal.

3.3. Algorithmic Differentiation and Scientific Computing

Participants: Alain Dervieux, Laurent Hascoët, Bruno Koobus.

linearization In Scientific Computing, the mathematical model often consists of Partial Differential Equations, that are discretized and then solved by a computer program. Linearization of these equations, or alternatively linearization of the computer program, predict the behavior of the model when small perturbations are applied. This is useful when the perturbations are effectively small, as in acoustics, or when one wants the sensitivity of the system with respect to one parameter, as in optimization.

adjoint state Consider a system of Partial Differential Equations that define some characteristics of a system with respect to some input parameters. Consider one particular scalar characteristic. Its sensitivity, (or gradient) with respect to the input parameters can be defined as the solution of "adjoint" equations, deduced from the original equations through linearization and transposition. The solution of the adjoint equations is known as the adjoint state.

Scientific Computing provides reliable simulations of complex systems. For example it is possible to *simulate* the steady or unsteady 3D air flow around a plane that captures the physical phenomena of shocks and turbulence. Next comes *optimization*, one degree higher in complexity because it repeatedly simulates and applies gradient-based optimization steps until an optimum is reached. The next sophistication is *robustness* i.e. to detect and to lower preference to a solution which, although maybe optimal, is very sensitive to uncertainty on design parameters or on manufacturing tolerances. This makes second derivative come into play. Similarly *Uncertainty Quantification* can use second derivatives to evaluate how uncertainty on the simulation inputs imply uncertainty on its outputs.

We investigate several approaches to obtain the gradient, between two extremes:

- One can write an *adjoint system* of mathematical equations, then discretize it and program it by hand. This is time consuming. Although this looks mathematically sound [32], this does not provide the gradient of the discretized function itself, thus degrading the final convergence of gradient-descent optimization.
- One can apply adjoint AD (*cf*3.1) on the program that discretizes and solves the direct system. This gives exactly the adjoint of the discrete function computed by the program. Theoretical results [31] guarantee convergence of these derivatives when the direct program converges. This approach is highly mechanizable, but leads to massive use of storage and may require code transformation by hand [36], [39] to reduce memory usage.

If for instance the model is steady, or when the computation uses a Fixed-Point iteration, tradeoffs exist between these two extremes [33], [27] that combine low storage consumption with possible automated adjoint generation. We advocate incorporating them into the AD model and into the AD tools.

GAMMA3 Project-Team (section vide)

GECO Project-Team

3. Research Program

3.1. Geometric control theory

The main research topic of the project-team is **geometric control**, with a special focus on **control design**. The application areas that we target are control of quantum mechanical systems, neurogeometry and switched systems.

Geometric control theory provides a viewpoint and several tools, issued in particular from differential geometry, to tackle typical questions arising in the control framework: controllability, observability, stabilization, optimal control... [22], [56] The geometric control approach is particularly well suited for systems involving nonlinear and nonholonomic phenomena. We recall that nonholonomicity refers to the property of a velocity constraint that is not equivalent to a state constraint.

The expression **control design** refers here to all phases of the construction of a control law, in a mainly open-loop perspective: modeling, controllability analysis, output tracking, motion planning, simultaneous control algorithms, tracking algorithms, performance comparisons for control and tracking algorithms, simulation and implementation.

We recall that

- **controllability** denotes the property of a system for which any two states can be connected by a trajectory corresponding to an admissible control law ;
- **output tracking** refers to a control strategy aiming at keeping the value of some functions of the state arbitrarily close to a prescribed time-dependent profile. A typical example is **configuration tracking** for a mechanical system, in which the controls act as forces and one prescribes the position variables along the trajectory, while the evolution of the momenta is free. One can think for instance at the lateral movement of a car-like vehicle: even if such a movement is unfeasible, it can be tracked with arbitrary precision by applying a suitable control strategy;
- **motion planning** is the expression usually denoting the algorithmic strategy for selecting one control law steering the system from a given initial state to an attainable final one;
- **simultaneous control** concerns algorithms that aim at driving the system from two different initial conditions, with the same control law and over the same time interval, towards two given final states (one can think, for instance, at some control action on a fluid whose goal is to steer simultaneously two floating bodies.) Clearly, the study of which pairs (or n-uples) of states can be simultaneously connected thanks to an admissible control requires an additional controllability analysis with respect to the plain controllability mentioned above.

At the core of control design is then the notion of motion planning. Among the motion planning methods, a preeminent role is played by those based on the Lie algebra associated with the control system ([76], [63], [69]), those exploiting the possible flatness of the system ([50]) and those based on the continuation method ([88]). Optimal control is clearly another method for choosing a control law connecting two states, although it generally introduces new computational and theoretical difficulties.

Control systems with special structure, which are very important for applications are those for which the controls appear linearly. When the controls are not bounded, this means that the admissible velocities form a distribution in the tangent bundle to the state manifold. If the distribution is equipped with a smoothly varying norm (representing a cost of the control), the resulting geometrical structure is called *sub-Riemannian*. Sub-Riemannian geometry thus appears as the underlying geometry of the nonholonomic control systems, playing the same role as Euclidean geometry for linear systems. As such, its study is fundamental for control design. Moreover its importance goes far beyond control theory and is an active field of research both in differential geometry ([75]), geometric measure theory ([51], [26]) and hypoelliptic operator theory ([38]).

Other important classes of control systems are those modeling mechanical systems. The dynamics are naturally defined on the tangent or cotangent bundle of the configuration manifold, they have Lagrangian or Hamiltonian structure, and the controls act as forces. When the controls appear linearly, the resulting model can be seen somehow as a second-order sub-Riemannian structure (see [43]).

The control design topics presented above naturally extend to the case of distributed parameter control systems. The geometric approach to control systems governed by partial differential equations is a novel subject with great potential. It could complement purely analytical and numerical approaches, thanks to its more dynamical, qualitative and intrinsic point of view. An interesting example of this approach is the paper [23] about the controllability of Navier–Stokes equation by low forcing modes.

GEOSTAT Project-Team

3. Research Program

3.1. Multiscale description in terms of multiplicative cascade

GEOSTAT is studying complex signals under the point of view of methods developed in *statistical physics* to study complex systems, with a strong emphasis on multiresolution analysis. Linear methods in signal processing refer to the standard point of view under which operators are expressed by simple convolutions with impulse responses. Linear methods in signal processing are widely used, from least-square deconvolution methods in adaptive optics to source-filter models in speech processing. Because of the absence of localization of the Fourier transform, linear methods are not successful to unlock the multiscale structures and cascading properties of variables which are of primary importance as stated by the physics of the phenomena. This is the reason why new approaches, such as DFA (Detrented Fluctuation Analysis), Time-frequency analysis, variations on curvelets [45] etc. have appeared during the last decades. Recent advances in dimensionality reduction, and notably in Compressive Sensing, go beyond the Nyquist rate in sampling theory using nonlinear reconstruction, but data reduction occur at random places, independently of geometric localization of information content, which can be very useful for acquisition purposes, but of lower impact in signal analysis. One important result obtained in GEOSTAT is the effective use of multiresolution analysis associated to optimal inference along the scales of a complex system. The multiresolution analysis is performed on dimensionless quantities given by the *singularity exponents* which encode properly the geometrical structures associated to multiscale organization. This is applied successfully in the derivation of high resolution ocean dynamics, or the high resolution mapping of gaseous exchanges between the ocean and the atmosphere; the latter is of primary importance for a quantitative evaluation of global warming. Understanding the dynamics of complex systems is recognized as a new discipline, which makes use of theoretical and methodological foundations coming from nonlinear physics, the study of dynamical systems and many aspects of computer science. One of the challenges is related to the question of *emergence* in complex systems: large-scale effects measurable macroscopically from a system made of huge numbers of interactive agents [36], [33], [50], [40]. Some quantities related to nonlinearity, such as Lyapunov exponents, Kolmogorov-Sinai entropy etc. can be computed at least in the phase space [34]. Consequently, knowledge from acquisitions of complex systems (which include *complex signals*) could be obtained from information about the phase space. A result from F. Takens [46] about strange attractors in turbulence has motivated the determination of discrete dynamical systems associated to time series [38], and consequently the theoretical determination of nonlinear characteristics associated to complex acquisitions. Emergence phenomena can also be traced inside complex signals themselves, by trying to localize information content geometrically. Fundamentally, in the nonlinear analysis of complex signals there are broadly two approaches: characterization by attractors (embedding and bifurcation) and time-frequency, multiscale/multiresolution approaches. Time-frequency analysis [35] and multiscale/multiresolution are the subjects of intense research and are profoundly reshaping the analysis of complex signals by nonlinear approaches [32], [37]. In real situations, the phase space associated to the acquisition of a complex phenomenon is unknown. It is however possible to relate, inside the signal's domain, local predictability to local reconstruction and deduce from that singularity exponents [11] [7]. We are working on:

- the determination of quantities related to universality classses,
- the geometric localization of multiscale properties in complex signals,
- cascading characteristics of physical variables.

The alternative approach taken in GEOSTAT is microscopical, or geometrical: the multiscale structures which have their "fingerprint" in complex signals are being isolated in a single realization of the complex system, i.e. using the data of the signal itself, as opposed to the consideration of grand ensembles or a wide set of realizations. This is much harder than the ergodic approaches, but it is possible because a reconstruction formula such as the one derived in [47] is local and reconstruction in the signal's domain is related to predictability. This approach is analogous to the consideration of "microcanonical ensembles" in statistical mechanics.

A multiscale organization is a fundamental feature of a complex system, it can be for example related to the cascading properties in turbulent systems. We make use of this kind of description when analyzing turbulent signals: intermittency is observed within the inertial range and is related to the fact that, in the case of FDT, symmetry is restored only in a statistical sense, a fact that has consequences on the quality of any nonlinear signal representation by frames or dictionaries.

The example of FDT as a standard "template" for developing general methods that apply to a vast class of complex systems and signals is of fundamental interest because, in FDT, the existence of a multiscale hierarchy $\mathcal{F}_h$ which is of multifractal nature and geometrically localized can be derived from physical considerations. This geometric hierarchy of sets is responsible for the shape of the computed singularity spectra, which in turn is related to the statistical organization of information content in a signal. It explains scale invariance, a characteristic feature of complex signals. The analogy from statistical physics comes from the fact that singularity exponents are direct generalizations of *critical exponents* which explain the macroscopic properties of a system around critical points, and the quantitative characterization of *universality classes*, which allow the definition of methods and algorithms that apply to general complex signals and systems, and not only turbulent signals: signals which belong to a same universality class share common statistical organization. In GEOSTAT, the approach to singularity exponents is done within a microcanonical setting, which can interestingly be compared with other approaches such that wavelet leaders, WTMM or DFA. During the past decades, classical approaches (here called "canonical" because they use the analogy taken from the consideration of "canonical ensembles" in statistical mechanics) permitted the development of a well-established analogy taken from thermodynamics in the analysis of complex signals: if $\mathcal{F}$ is the free energy, $\mathcal{T}$ the temperature measured in energy units, $\mathcal{U}$ the internal energy per volume unit $\mathcal{S}$ the entropy and $\widehat{\beta} = 1/\mathcal{T}$, then the scaling exponents associated to moments of intensive variables $p \rightarrow \tau_p$ corresponds to $\widehat{\beta}\mathcal{F}$, $\mathcal{U}(\widehat{\beta})$ corresponds to the singularity exponents values, and $\mathcal{S}(\mathcal{U})$ to the singularity spectrum.

The singularity exponents belong to a universality class, independently of microscopic properties in the phase space of various complex systems, and beyond the particular case of turbulent data (where the existence of a multiscale hierarchy, of multifractal nature, can be inferred directly from physical considerations). They describe common multiscale statistical organizations in different complex systems [44], and this is why GEOSTAT is working on nonlinear signal processing tools that are applied to very different types of signals.

For example we give some insight about the collaboration with LEGOS Dynbio team [0] about high-resolution ocean dynamics from microcanonical formulations in nonlinear complex signal analysis. Indeed, synoptic determination of ocean circulation using data acquired from space, with a coherent depiction of its turbulent characteristics remains a fundamental challenge in oceanography. This determination has the potential of revealing all aspects of the ocean dynamic variability on a wide range of spatio-temporal scales and will enhance our understanding of ocean-atmosphere exchanges at super resolution, as required in the present context of climate change. We show that the determination of a multiresolution analysis associated to the multiplicative cascade of a typical physical variable like the Sea Surface Temperature permits an *optimal inference* of oceanic motion field across the scales, resulting in a new method for deriving super resolution oceanic motion from lower resolution altimetry data; the resulting oceanic motion field is validated at super resolution with the use of Lagrangian buoy data available from the Global Drifter Program [0]. In FDT, singularity exponents range in a bounded interval: $]h_\infty, h_{\max}[$ with $h_\infty < 0$ being the most singular exponent. Points $\mathbf{r}$ for which $h(\mathbf{r}) < 0$ localize the stongest transitions in the turbulent fluid, where an intensive

[0] http://www.legos.obs-mip.fr/recherches/equipes/dynbio.

[0] http://www.aoml.noaa.gov/phod/dac/index.php.

physical variable like sea surface temperature behaves like $1/\mathbf{r}^{|h(\mathbf{r})|}$. The links between the geometricaly localized singularity exponents, the scaling exponents of structure functions, the multiplicative cascade and the multiscale hierarchy $\mathcal{F}_h$ is the following:

$$\begin{cases} \mathcal{F}_h = \{\mathbf{r} \ \mid \ h(\mathbf{r}) = h\} \\ D(h) = \dim \mathcal{F}_h \\ \tau_p = \inf_h \{ph + 3 - D(h)\} \\ D(h) = \inf_p \{ph + 3 - \tau_p\} \end{cases} \tag{7}$$

Let $\mathfrak{S}(\mathbf{x})$ be the bidimensionnal signal recording, for each sample point $\mathbf{x}$ representing a pixel on the surface of the ocean of given resolution, the sea surface temperature (sst). To this signal we associate a measure μ whose density w.r.t Lebesgue measure is the signal's gradient norm, and from which the singularity exponents are computed [6]. It is fundamental to notice here that, contrary to other types of exponents computed in Oceanography, such as Finite Size Lyapunov exponents, singularity exponents are computed at instantaneous time, and do not need time series.

Having computed the singularity exponents at each point of a SST signal, a microcanonical version of the multiplicative cascade associated to the scaling properties of the sst become available. The idea of the existence of a geometrically localized multiplicative cascade goes back to [43]. The multiplicative cascade, written pointwise, introduces random variables $\eta_{l'/l}(\mathbf{x})$ for $0 < l' < l$ such that

$$\mathcal{T}_\psi \mu(\mathbf{x}, l') \ = \ \eta_{l'/l}(\mathbf{x}) \mathcal{T}_\psi \mu(\mathbf{x}, l) \tag{8}$$

in which the equality is valid pointwise and not only in distribution. Any mother wavelet ψ such that the process $\eta_{l'/l}(\mathbf{x})$ is independant of $\mathcal{T}_\psi \mu(\mathbf{x}, l')$ is called an optimal wavelet: it optimizes inference of physical variables across the scales and consequently describes the multiplicative cascade at each point $\mathbf{x}$ in the signal domain. The injection variables $\eta_{l'/l}(\mathbf{x})$ are indefinitely divisible: $\eta_k(\mathbf{x})\eta_{k'}(\mathbf{x}) \doteq \eta_{kk'}(\mathbf{x})$. It is possible to optimize cross-scale inference of physical variables by considering a *multiresolution analysis* associated to a discrete covering of the "space-frequency" domain. Denoting as usual $(V_j)_{j \in \mathbb{Z}}$ and $(W_j)_{j \in \mathbb{Z}}$ the discrete sequence of approximation and detail spaces associated to a given scaling function, and denoting by $\psi \in L^2(\mathbb{R}^2)$ a wavelet which generates an Hilbertian basis on each detail space W_j, it is known that the detail spaces encode borders and transition information, which is ideally described in the case of turbulent signals by the singularity exponents $\mathbf{h}(\mathbf{x})$. Consequently, a novel idea for super-resolution consists in computing a multiresolution analysis on the signal of singularity exponents $\mathbf{h}(\mathbf{x})$, and to consider that the detail information coming from spaces W_j is given the signal $\mathbf{h}(\mathbf{x})$. The associated orthogonal projection $\pi_j : L^2(\mathbb{R}^2) \rightarrow W_j$ defined by $\pi_j(\mathbf{h}) = \sum_{n \in \mathbb{Z}} \langle \ \mathbf{h} \mid \psi_{j,n} \ \rangle \psi_{j,n}$ is then used in the reconstruction formula for retrieving a physical variable at higher resolution from its low resolution counterpart. If $\mathfrak{S}(\mathbf{x})$ is such a variable, we use a reconstruction formula: $A_{j-1}\mathfrak{S} = A_j \mathfrak{S} + \pi_j(\mathbf{h})$ with $A_j : L^2(\mathbb{R}^2) \rightarrow V_j$ is the orthogonal projection on the space V_j (approximation operator) and π_j is the orthogonal projection on the detail spaces W_j associated to the signal of singularity exponents $\mathbf{h}(\mathbf{x})$. Validation is performed using Lagrangian buoy data with very good results [10]. We have realized a demonstration movie showing the turbulent ocean dynamics at an SST resolution of 4 km computed from the SST microcanonical cascade and the low-resolution GEKCO product for the year 2006 over the southwestern part of the Indian Ocean. We replace the missing data in the SST MODIS product (clouds and satellite swath) by the corresponding data available from the Operational SST and Sea Ice Analysis (OSTIA) provided by the Group for High-Resolution SST Project [11], which, however, is of lower quality. Two images per day are generated for the whole year of 2006. The resulting images show the norm of the vector field in the background rendered using the line integral convolution algorithm. In the foreground, we show the resulting vector field in a linear gray-scale color map. See link to movie (size: 800 Mo).

3.2. Excitable systems and heartbeat signal analysis

We are developing novel approaches to heartbeat signal analysis for understanding chronic atrial fibrillation. The noisy aspect of data recorded by electrodes, on the inner surface of human atria during episodes of atrial fibrillation, exhibit intriguing features for excitable media. Instead of phase chaos as typically expected, it shares many common traits of non-equilibrium fluctuations in disordered systems or strong turbulence. To assess those peculiar observations we investigate a *synaptic plasticity* that affects conduction properties. Electrical synapses comprise many different kinds of connexins, which may be affected by diverse factors, so we use a generic approach. Slight detuning of their linear response leads to an instability of the modulating agents, here an excess charge. Acting on slow time scales of repolarisation, it is understood as *collective modes* propagating through and retroacting on each synapse: the medium is *desynchronised*. It is not a syncytium. We propose to associate transient states with a phenomenon called *electrical remodelling*, which has not received any accepted description thus far. Moreover, from the properties of the model it is possible to start exploring phase space. Transitions between different regimes could help decipher stages in the evolution of the disease from acute to chronic, one main goal of cardiovascular research.

Theoretically, a myocardium is an excitable tissue acting under normal circumstances as a functional syncytium of myocardial cells. Models of excitability for the heart are reaction-diffusion systems describing the propagation of electric pulses called action potentials similarly to models for axons. Reaction results from ionic exchange cycles between the cytoplasm of excitable cells and their extra-cellular medium, when initiated by a stimulus above some threshold. Pulses are robust topological structures.

Considering the stable fixed point as a phase resetting state, chaos may arise in spatio-temporal sequences. This is the paradigm for cardiac fibrillation. But, it is incompatible with the following observations: the distributions of amplitudes all collapse on a scaling function G. We map exponents on data patients provided by IHU LIRYC showing non-universal properties. Singular exponents are observed with consistent Hausdorff dimension of sets $D(h)$. Negative contribution is high, suggesting an underlying multiplicative process.

Excess charge in cells like of *Ca* may perturb the dynamics of synapses. We consider a physiologically plausible linear response of synapses to the electro-chemical potential. This response is unknown as of today. The new dynamics may interact with excitability. It has the specific form of a Rayleigh instability. Cycles become retarded or advanced. Hopf bifurcation and chaos are allowed creating EADs (Early After Depolarization). Regarding propagation, pulses are pinned and released on a chaotic background. Cycle modulations create defects via facilitation through the third dimension. Defects proliferate creating a glassy phase, which back-scatter fronts in 1D and roughens them in 2D. Further effective inhibitor diffusion splits them. Electrical remodelling is here the abnormal modification of the cell dynamics without any membrane alteration.

There are features of Self Organized Criticality (SOC) in large regions of phase space. Pulses have a phase and propagate on a random medium. For instance one paradigm we investigate would be:

$$\partial_t \theta + \sin(\theta + \widetilde{\phi}) = \Omega + \partial_{xx}\theta \tag{9}$$

(θ: phase of activation front, Ω: tachycardia frequency, $\widetilde{\phi}$: phase perturbation). Randomness reactualises nonlinearly, which tells that the noise is quenched and reset. For instance in 1 + 1D, spatio-temporal maps look very much like optimal directed paths along diagonals. In 1 + 2D, we are guessing that pulses do propagate in the (q)KPZ universality class, just as the remodelling front does. This class is only fractal, but together with large deviations of the fluctuations, it may be consistent with a multi-affine process. Physiologically, one interesting bonus is the interpretation of non-reentrant Tachycardia as dislocation patterns slowly evolving.

3.3. Speech analysis

Our research in speech processing focus on the development of novel nonlinear analysis methods for the characterization and classification of pathological and affective speech. For the latter, classical linear methods do not generally capture the nonlinearity, aperiodicity, turbulence and noise that can be present in pathological voices. We thus aim to design and extract new features that allow better characterization/classification of such voices, while being easy to interpret by clinicians. For the former, recent research have shown that the voice source signal information allow significant improvement of speech emotion detection systems. Our goal is to develop novel nonlinear techniques to extract relevant voice source features and to design efficient machine learning algorithms for robust emotion classification.

I4S Project-Team

3. Research Program

3.1. Vibration analysis

In this section, the main features for the key monitoring issues, namely identification, detection, and diagnostics, are provided, and a particular instantiation relevant for vibration monitoring is described.

It should be stressed that the foundations for identification, detection, and diagnostics, are fairly general, if not generic. Handling high order linear dynamical systems, in connection with finite elements models, which call for using subspace-based methods, is specific to vibration-based SHM. Actually, one particular feature of model-based sensor information data processing as exercised in I4S, is the combined use of black-box or semi-physical models together with physical ones. Black-box and semi-physical models are, for example, eigenstructure parameterizations of linear MIMO systems, of interest for modal analysis and vibration-based SHM. Such models are intended to be identifiable. However, due to the large model orders that need to be considered, the issue of model order selection is really a challenge. Traditional advanced techniques from statistics such as the various forms of Akaike criteria (AIC, BIC, MDL, ...) do not work at all. This gives rise to new research activities specific to handling high order models.

Our approach to monitoring assumes that a model of the monitored system is available. This is a reasonable assumption, especially within the SHM areas. The main feature of our monitoring method is its intrinsic ability to the early warning of small deviations of a system with respect to a reference (safe) behavior under usual operating conditions, namely without any artificial excitation or other external action. Such a normal behavior is summarized in a reference parameter vector θ_0, for example a collection of modes and mode-shapes.

3.1.1. Identification

The behavior of the monitored continuous system is assumed to be described by a parametric model $\{\mathbf{P}_\theta\, , \, \theta \in \Theta\}$, where the distribution of the observations $(Z_0, ..., Z_N)$ is characterized by the parameter vector $\theta \in \Theta$.

For reasons closely related to the vibrations monitoring applications, we have been investigating subspace-based methods, for both the identification and the monitoring of the eigenstructure (λ, ϕ_λ) of the state transition matrix F of a linear dynamical state-space system :

$$\left\{ \begin{array}{rcl} X_{k+1} & = & F \; X_k + V_{k+1} \\ Y_k & = & H \; X_k + W_k \end{array} \right. , \tag{10}$$

namely the $(\lambda, \varphi_\lambda)$ defined by :

$$\det \; (F - \lambda \; I) = 0, \quad (F - \lambda \; I) \; \phi_\lambda = 0, \quad \varphi_\lambda \stackrel{\Delta}{=} H \; \phi_\lambda \tag{11}$$

The (canonical) parameter vector in that case is :

$$\theta \stackrel{\Delta}{=} \left(\begin{array}{c} \Lambda \\ \mathrm{vec}\Phi \end{array} \right) \tag{12}$$

where Λ is the vector whose elements are the eigenvalues λ, Φ is the matrix whose columns are the φ_λ's, and vec is the column stacking operator.

Subspace-based methods is the generic name for linear systems identification algorithms based on either time domain measurements or output covariance matrices, in which different subspaces of Gaussian random vectors play a key role [54].

Let $R_i \triangleq \mathbf{E}\left(Y_k \; Y_{k-i}^T\right)$ and:

$$\mathcal{H}_{p+1,q} \triangleq \begin{pmatrix} R_1 & R_2 & \vdots & R_q \\ R_2 & R_3 & \vdots & R_{q+1} \\ \vdots & \vdots & \vdots & \vdots \\ R_{p+1} & R_{p+2} & \vdots & R_{p+q} \end{pmatrix} \triangleq \text{Hank}\left(R_i\right) \tag{13}$$

be the output covariance and Hankel matrices, respectively; and: $G \triangleq \mathbf{E}\left(X_k Y_{k-1}^T\right)$. Direct computations of the R_i's from the equations (4) lead to the well known key factorizations :

$$\begin{aligned} R_i &= HF^{i-1}G \\ \mathcal{H}_{p+1,q} &= \mathcal{O}_{p+1}(H,F) \; \mathcal{C}_q(F,G) \end{aligned} \tag{14}$$

where:

$$\mathcal{O}_{p+1}(H,F) \triangleq \begin{pmatrix} H \\ HF \\ \vdots \\ HF^p \end{pmatrix} \quad \text{and} \quad \mathcal{C}_q(F,G) \triangleq (G \; FG \; \cdots \; F^{q-1}G) \tag{15}$$

are the observability and controllability matrices, respectively. The observation matrix H is then found in the first block-row of the observability matrix $\mathcal{O}$. The state-transition matrix F is obtained from the shift invariance property of $\mathcal{O}$. The eigenstructure (λ, ϕ_λ) then results from (5).

Since the actual model order is generally not known, this procedure is run with increasing model orders.

3.1.2. Detection

Our approach to on-board detection is based on the so-called asymptotic statistical local approach. It is worth noticing that these investigations of ours have been initially motivated by a vibration monitoring application example. It should also be stressed that, as opposite to many monitoring approaches, our method does not require repeated identification for each newly collected data sample.

For achieving the early detection of small deviations with respect to the normal behavior, our approach generates, on the basis of the reference parameter vector θ_0 and a new data record, indicators which automatically perform :

- The early detection of a slight mismatch between the model and the data;
- A preliminary diagnostics and localization of the deviation(s);
- The tradeoff between the magnitude of the detected changes and the uncertainty resulting from the estimation error in the reference model and the measurement noise level.

These indicators are computationally cheap, and thus can be embedded. This is of particular interest in some applications, such as flutter monitoring.

Choosing the eigenvectors of matrix F as a basis for the state space of model (4) yields the following representation of the observability matrix:

$$\mathcal{O}_{p+1}(\theta) = \begin{pmatrix} \Phi \\ \Phi\Delta \\ \vdots \\ \Phi\Delta^p \end{pmatrix} \tag{16}$$

where $\Delta \triangleq \operatorname{diag}(\Lambda)$, and Λ and Φ are as in (6). Whether a nominal parameter θ_0 fits a given output covariance sequence $(R_j)_j$ is characterized by:

$$\mathcal{O}_{p+1}(\theta_0) \ \text{ and } \ \mathcal{H}_{p+1,q} \ \text{ have the same left kernel space.} \tag{17}$$

This property can be checked as follows. From the nominal θ_0, compute $\mathcal{O}_{p+1}(\theta_0)$ using (10), and perform e.g. a singular value decomposition (SVD) of $\mathcal{O}_{p+1}(\theta_0)$ for extracting a matrix U such that:

$$U^T\ U = I_s \ \text{ and } \ U^T\ \mathcal{O}_{p+1}(\theta_0) = 0 \tag{18}$$

Matrix U is not unique (two such matrices relate through a post-multiplication with an orthonormal matrix), but can be regarded as a function of θ_0. Then the characterization writes:

$$U(\theta_0)^T\ \mathcal{H}_{p+1,q} = 0 \tag{19}$$

3.1.2.1. Residual associated with subspace identification.

Assume now that *a reference* θ_0 *and a new sample* $Y_1, \cdots, Y_N$ *are available.* For checking whether the data agree with θ_0, the idea is to compute the empirical Hankel matrix $\widehat{\mathcal{H}}_{p+1,q}$:

$$\widehat{\mathcal{H}}_{p+1,q} \triangleq \text{Hank}\left(\widehat{R}_i\right), \quad \widehat{R}_i \triangleq 1/(N-i) \sum_{k=i+1}^{N} Y_k\ Y_{k-i}^T \tag{20}$$

and to define the residual vector:

$$\zeta_N(\theta_0) \triangleq \sqrt{N}\ \text{vec}\left(U(\theta_0)^T\ \widehat{\mathcal{H}}_{p+1,q}\right) \tag{21}$$

Let θ be the actual parameter value for the system which generated the new data sample, and $\mathbf{E}_\theta$ be the expectation when the actual system parameter is θ. From (13), we know that $\zeta_N(\theta_0)$ has zero mean when no change occurs in θ, and nonzero mean if a change occurs. Thus $\zeta_N(\theta_0)$ plays the role of a residual.

As in most fault detection approaches, the key issue is to design a *residual*, which is ideally close to zero under normal operation, and has low sensitivity to noises and other nuisance perturbations, but high sensitivity to small deviations, before they develop into events to be avoided (damages, faults, ...). The originality of our approach is to :

- *Design* the residual basically as a *parameter estimating function*,
- *Evaluate* the residual thanks to a kind of central limit theorem, stating that the residual is asymptotically Gaussian and reflects the presence of a deviation in the parameter vector through a change in its own mean vector, which switches from zero in the reference situation to a non-zero value.

The central limit theorem shows [48] that the residual is asymptotically Gaussian :

$$\zeta_N \xrightarrow[N \to \infty]{} \begin{cases} \mathcal{N}(0, \Sigma) & \text{under } \mathbf{P}_{\theta_0} \ , \\ \\ \mathcal{N}(\mathcal{J}\,\eta, \Sigma) & \text{under } \mathbf{P}_{\theta_0+\eta/\sqrt{N}} \ , \end{cases} \tag{22}$$

where the asymptotic covariance matrix Σ can be estimated, and manifests the deviation in the parameter vector by a change in its own mean value. Then, deciding between $\eta = 0$ and $\eta \neq 0$ amounts to compute the following χ^2-test, provided that $\mathcal{J}$ is full rank and Σ is invertible :

$$\chi^2 = \bar{\zeta}^T \, \mathbf{F}^{-1} \, \bar{\zeta} \gtrless \lambda \ . \tag{23}$$

where

$$\bar{\zeta} \triangleq \mathcal{J}^T \, \Sigma^{-1} \, \zeta_N \quad \text{and} \quad \mathbf{F} \triangleq \mathcal{J}^T \, \Sigma^{-1} \, \mathcal{J} \tag{24}$$

3.1.3. Diagnostics

A further monitoring step, often called *fault isolation*, consists in determining which (subsets of) components of the parameter vector θ have been affected by the change. Solutions for that are now described. How this relates to diagnostics is addressed afterwards.

The question: *which (subsets of) components of θ have changed ?*, can be addressed using either nuisance parameters elimination methods or a multiple hypotheses testing approach [47].

In most SHM applications, a complex physical system, characterized by a generally non identifiable parameter vector Φ has to be monitored using a simple (black-box) model characterized by an identifiable parameter vector θ. A typical example is the vibration monitoring problem for which complex finite elements models are often available but not identifiable, whereas the small number of existing sensors calls for identifying only simplified input-output (black-box) representations. In such a situation, two different diagnosis problems may arise, namely diagnosis in terms of the black-box parameter θ and diagnosis in terms of the parameter vector Φ of the underlying physical model.

The isolation methods sketched above are possible solutions to the former. Our approach to the latter diagnosis problem is basically a detection approach again, and not a (generally ill-posed) inverse problem estimation approach.

The basic idea is to note that the physical sensitivity matrix writes $\mathcal{J} \, \mathcal{J}_{\Phi\theta}$, where $\mathcal{J}_{\Phi\theta}$ is the Jacobian matrix at Φ_0 of the application $\Phi \mapsto \theta(\Phi)$, and to use the sensitivity test for the components of the parameter vector Φ. Typically this results in the following type of directional test :

$$\chi^2_\Phi = \zeta^T \, \Sigma^{-1} \, \mathcal{J} \, \mathcal{J}_{\Phi\theta} \, (\mathcal{J}^T_{\Phi\theta} \, \mathcal{J}^T \, \Sigma^{-1} \, \mathcal{J} \, \mathcal{J}_{\Phi\theta})^{-1} \, \mathcal{J}^T_{\Phi\theta} \, \mathcal{J}^T \, \Sigma^{-1} \, \zeta \gtrless \lambda \ . \tag{25}$$

It should be clear that the selection of a particular parameterization Φ for the physical model may have a non negligible influence on such type of tests, according to the numerical conditioning of the Jacobian matrices $\mathcal{J}_{\Phi\theta}$.

3.2. Thermal methods

3.2.1. Infrared thermography and heat transfer

This section introduce the infrared radiation and its link with the temperature, in the next part different measurement methods based on that principle are presented.

3.2.1.1. Infrared radiation

Infrared is an electromagnetic radiation having a wavelength between $0.2\mu m$ and $1\ mm$, this range begin in uv spectrum and it ends on the microwaves domain, see Figure 1 .

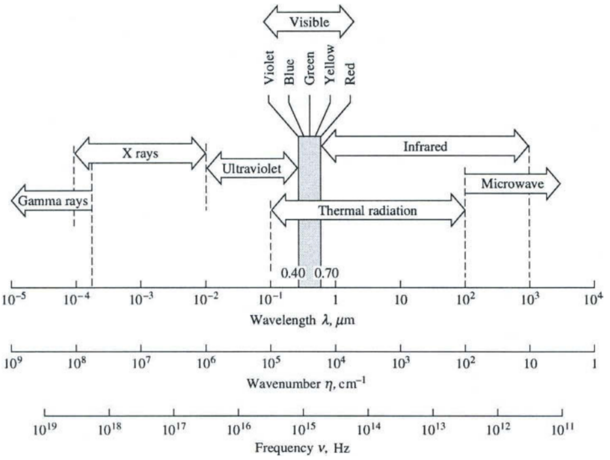


Figure 1. Electromagnetic spectrum - Credit MODEST, M.F. (1993). Radiative Heat Transfer. Academic Press.

For scientific purpose infrared can be divided in three ranges of wavelength in which the application varies, see Table 1 .

Table 1. Wavelength bands in the infrared according to ISO 20473:2007

Band name	**wavelength**	**Uses $\setminus$ definition**
Near infrared (PIR, IR-A, NIR)	$0.7 - 3\mu$m	Reflected solar heat flux
Mid infrared (MIR, IR-B)	$3 - 50\mu$m	Thermal infrared
Far infrared (LIR, IR-C, FIR)	$50 - 1000\mu$m	Astronomy

Our work is concentrated in the mid infrared spectral band. Keep in mind that Table 1 represents the ISO 20473 division scheme, in the literature boundaries between bands can move slightly.

The Plank's law, proposed by Max Planck en 1901, allow to compute the black body emission spectrum for various temperatures (and only temperatures), see Figure 2 left. The black body is a theoretical construction, it represents perfect energy emitter at a given temperature, cf Equation (20).

$$M^{o}_{\lambda,T} = \frac{C_1 \lambda^{-5}}{\exp^{\frac{C_2}{\lambda T}} - 1} \tag{26}$$

With λ the wavelength in m and T as the temperature in Kelvin. The C_1 an C_2 constant, respectively in W.m^2 and m.K are defined as follow:

$$\begin{aligned} C_1 &= 2hc^2\pi \\ C_2 &= h\frac{c}{k} \end{aligned} \tag{27}$$

with

- c The electromagnetic wave speed (in vacuum c is the light speed in m.s^{-1}).
- $k = 1.381e^{-23}$ J.K^{-1} The Boltzmann (Entropy definition from Ludwig Boltzmann 1873). It can be seen as a proportionality factor between the temperature and the energy of a system.
- $h \approx 6,62606957e^{-34}$ J.s The Plank constant. It is the link between the photons energy and their frequency.

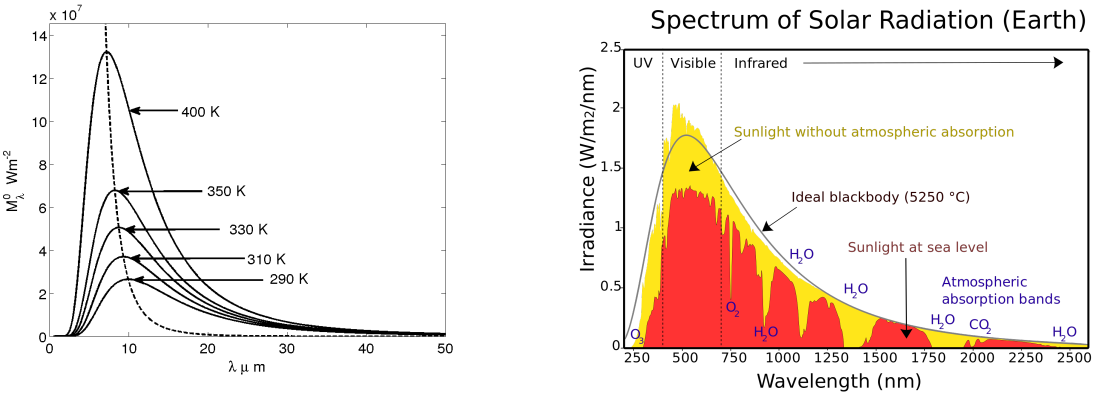


Figure 2. Left: Plank's law at various temperatures - Right: Energy spectrum of the atmosphere

By generalizing the Plank's law with the Stefan Boltzmann law (proposed first in 1879 and then in 1884 by Joseph Stefan and Ludwig Boltzmann) it is possible to address mathematically the energy spectrum of real body at each wavelength dependent of the temperature, the optical condition and the real body properties, which is the base of the infrared thermography.

For example, Figure 2 right presents the energy spectrum of the atmosphere at various levels, it can be seen that the various properties of the atmosphere affect the spectrum at various wavelengths. Other important point is that the infrared solar heat flux can be approximated by a black body at 5523,15 K.

3.2.1.2. Infrared Thermography

The infrared thermography is a way to measure the thermal radiation received from a medium. With that information about the electromagnetic flux it is possible to estimate the surface temperature of the body, see section 3.2.1.1 . Various types of detector can assure the measure of the electromagnetic radiation.

Those different detectors can take various forms and/or manufacturing process. For our research purpose we use uncooled infrared camera using a matrix of microbolometers detectors. A microbolometer, as a lot of transducers, converts a radiation in electric current used to represent the physical quantity (here the heat flux).

This field of activity includes the use and the improvement of vision system, like in [3].

3.2.2. Heat transfer theory

Once the acquisition process is done, it is useful to model the heat conduction inside the cartesian domain Ω. Note that in opaque solid medium the heat conduction is the only mode of heat transfer. Proposed by Jean Baptiste Biot in 1804 and experimentally demonstrated by Joseph Fourier in 1821, the Fourier Law describes the heat flux inside a solid, cf Equation (22).

$$\varphi = k\nabla T \quad X \in \Omega \tag{28}$$

Where k is the thermal conductivity in W.m^{-1}.K ^{o}, ∇ is the gradient operator and φ is the heat flux density in Wm^{-2}. This law illustrates the first principle of thermodynamic (law of conservation of energy) and implies the second principle (irreversibility of the phenomenon), from this law it can be seen that the heat flux always goes from hot area to cold area.

An energy balance with respect to the first principle drives to the expression of the heat conduction in all point of the domain Ω, cf Equation (23). This equation has been proposed by Joseph Fourier in 1811.

$$\rho C \frac{\partial T(X,t)}{\partial t} = \nabla \cdot (k \nabla T) + P \quad X \in \Omega \tag{29}$$

With $\nabla.()$ the divergence operator, C the specific heat capacity in J.kg^{-1}.^{o}K^{-1}, ρ the volumetric mass density in kg. m^{-3}, X the space variable $X = \{x, y, z\}$ and P a possible internal heat production in W.m^{-3}.

To solve the system (23), it is necessary to express the boundaries conditions of the system. With the developments presented in section 3.2.1.1 and the Fourier's law it is possible, for example, to express the thermal radiation and the convection phenomenon which can occur at $\partial\Omega$ the system boundaries, cf Equation (24).

$$\varphi = k \nabla T \cdot n = \underbrace{h \left(T_{fluid} - T_{Boundarie} \right)}_{\text{Convection}} + \underbrace{\epsilon \sigma_s \left(T^4_{environement} - T^4_{Boundary} \right)}_{\text{Radiation}} + \varphi_0 \quad X \in \partial\Omega \tag{30}$$

Equation (24) is the so called Robin condition on the boundary $\partial\Omega$, where n is the normal, h the convective heat transfer coefficient in W.m^{-2}.K^{-1} and φ_0 an external energy contribution W.m^{-2}, in cases where the external energy contribution is artificial and controlled we call it active thermography (spotlight etc...) in the contrary it is called passive thermography (direct solar heat flux).

The systems presented in the different sections above (3.2.1 to 3.2.2) are useful to build physical models in order to represents the measured quantity. To estimate key parameters, as the conductivity, one way to do is the model inversion, the next section will introduce that principle.

3.2.3. Inverse model for parameters estimation

Lets take any model A which can for example represent the conductive heat transfer in a medium, the model is solved for a parameter vector P and it results another vector b, cf Equation (25). For example if A represents the heat transfer, b can be the temperature evolution.

$$AP = b \tag{31}$$

With A a matrix of size $n \times m$, P a vector of size m and b of size n, preferentially $n >> P$. This model is called direct model, the inverse model consist to find a vector P which satisfy the results b of the direct model. For that we need to inverse the matrix A, cf Equation (26).

$$P = A^{-1} b \tag{32}$$

Here we want find the solution AP which is closest to the acquired measures M, Equation (27).

$$AP \approx \mathcal{M} \tag{33}$$

To do that it is important to respect the well posed condition established by Jacques Hadamard in 1902

- A solution exists.
- The solution is unique.
- The solution's behavior changes continuously with the initial conditions.

Unfortunately those condition are rarely respected in our field of study. That is why we dont solve directly the system (27) but we minimise the quadratic coast function (28) which represents the Legendre-Gauss least square algorithm for linear problems.

$$min_P \left(\|AP - \mathcal{M}\|^2 \right) = min_P \left(\mathcal{F} \right) \tag{34}$$

Where $\mathcal{F}$ can be a product of matrix.

$$\mathcal{F} = \left[AP - \mathcal{M}\right]^T \left[AP - \mathcal{M}\right] \tag{35}$$

In some case the problem is still ill-posed and need to be regularized for example using the Tikhonov regularization. An elegant way to minimize the cost function $\mathcal{F}$ is compute the gradient, Equation (30) and find where it is equal to zero.

$$\nabla\mathcal{F}(P) = 2\left[-\frac{\partial AP^T}{\partial P}\right]\left[AP - \mathcal{M}\right] = 2J(P)^T \left[AP - \mathcal{M}\right] \tag{36}$$

Where J is the sensitivity matrix of the model A to its parameter vector P.
Until now the inverse method proposed is valid only when the model A is linearly dependent of its parameter P, for the heat equation it is the case when you want to estimate the external heat flux, φ_0 in equation 24 . For all the other parameters, like the conductivity k the model is non-linearly dependant of its parameter P. For such case the use of iterative algorithm is needed, for example the Levenberg-Marquardt algorithm, cf Equation (31).

$$P^{k+1} = P^k + \left[(J^k)^T J^k + \mu^k \Omega^k\right]^{-1} (J^k)^T \left[\mathcal{M} - A(P^k)\right] \tag{37}$$

Equation (31) is solved iteratively at each loop k. Some of our results with such linear or non linear method can be seen in [4] or [2], more specifically [1] is a custom implementation of the Levenberg-Marquardt algorithm based on the adjoint method (developed by Jacques Louis Lions in 1968) coupled to the conjugate gradient algorithm to estimate wide properties field in a medium.

3.3. Reflectometry-based methods for electrical engineering and for civil engineering

The fast development of electronic devices in modern engineering systems involves more and more connections through cables, and consequently, with an increasing number connexion failures. Wires and connectors are subject to ageing and degradation, sometimes under severe environmental conditions. In many applications, the reliability of electrical connexions is related to the quality of production or service, whereas in critical applications reliability becomes also a safety issue. It is thus important to design smart diagnosis systems able to detect connection defects in real time. This fact has motivated research projects on methods for fault diagnosis in this field. Some of these projects are based on techniques of reflectometry, which consist in injecting waves into a cable or a network and in analyzing the reflections, as in the example of cable hard fault diagnosis. Depending on the injected waveforms and on the methods of analysis, various techniques of reflectometry are available. They all have the common advantage of being non destructive.

At Inria the research activities on reflectometry started within the SISYPHE EPI several years ago and now continue in the I4S EPI. Our most notable contribution in this area is a method based on the *inverse scattering* theory for the computation of *distributed characteristic impedance* along a cable from reflectometry measurements [14], [11], [53]. It provides an efficient solution for the diagnosis of *soft* faults in electrical cables, like in the example illustrated in Figure 3 . While most reflectometry methods for fault diagnosis are based on the detection and localization of impedance discontinuity, our method yielding the spatial profile of the characteristic impedance is particularly suitable for the diagnosis of soft faults *with no or weak impedance discontinuities*.

Fault diagnosis for wired networks have also been studied in Inria [55], [51]. The main results concern, on the one hand, simple star-shaped networks from measurements made at a single node, on the other hand, complex networks of arbitrary topological structure with complete node observations.

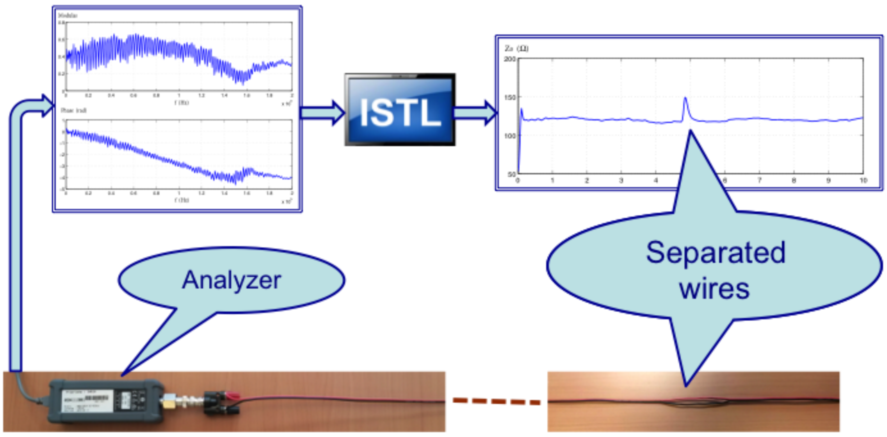


Figure 3. Inverse scattering software (ISTL) for cable soft fault diagnosis.

Though initially our studies on reflectometry were aiming at applications in electrical engineering, through our collaboration with IFSTTAR, we are also investigating applications in the field of civil engineering, by using electrical cables as sensors for monitoring changes in mechanical structures.

What follows is about some basic elements on mathematical equations of electric cables and networks, the main approach we follow in our study, and our future research directions.

3.3.1. Mathematical model of electric cables and networks

A cable excited by a signal generator can be characterized by the telegrapher's equations [52]

$$\begin{aligned}\frac{\partial}{\partial z}V(t,z) + L(z)\frac{\partial}{\partial t}I(t,z) + R(z)I(t,z) = 0\\ \frac{\partial}{\partial z}I(t,z) + C(z)\frac{\partial}{\partial t}V(t,z) + G(z)V(t,z) = 0\end{aligned} \tag{38}$$

where t represents the time, z is the longitudinal coordinate along the cable, $V(t,z)$ and $I(t,z)$ are respectively the voltage and the current in the cable at the time instant t and at the position z, $R(z), L(z), C(z)$ and $G(z)$ denote respectively the series resistance, the inductance, the capacitance and the shunt conductance per unit length of the cable at the position z. The left end of the cable (corresponding to $z = a$) is connected to a voltage source $V_s(t)$ with internal impedance R_s. The quantities $V_s(t)$, R_s, $V(t,a)$ and $I(t,a)$ are related by

$$V(t,a) = V_s(t) - R_s I(t,a). \tag{39}$$

At the right end of the cable (corresponding to $z = b$), the cable is connected to a load of impedance R_L, such that

$$V(t,b) \quad = R_L I(t,b). \tag{40}$$

One way for deriving the above model is to spatially discretize the cable and to characterize each small segment with 4 basic lumped parameter elements for the j-th segment: a resistance ΔR_j, an inductance ΔL_j, a capacitance ΔC_j and a conductance ΔG_j. The entire circuit is described by a system of ordinary differential equations. When the spatial discretization step size tends to zero, the limiting model leads to the telegrapher's equations (32).

A wired network is a set of cables connected at some nodes, where loads and sources can also be connected. Within each cable the current and voltage satisfy the telegrapher's equations (32), whereas at each node the current and voltage satisfy the Kirchhoff's laws, unless in case of connector failures.

3.3.2. The inverse scattering theory applied to cables

The inverse scattering transform was developed during the 1970s-1980s for the analysis of some nonlinear partial differential equations [50]. The visionary idea of applying this theory to solving the cable inverse problem goes also back to the 1980s [49]. After having completed some theoretic results directly linked to practice [14], [53], we started to successfully apply the inverse scattering theory to cable soft fault diagnosis, in collaboration with GEEPS-SUPELEC [11].

To link electric cables to the inverse scattering theory, the telegrapher's equations (32) are transformed in a few steps to fit into a particular form studied in the inverse scattering theory. The Fourier transform is first applied to transform the time domain model (32) into the frequency domain, the spatial coordinate z is then replaced by the propagation time

$$x(z) = \int_0^z \sqrt{L(s)C(s)}ds$$

and the frequency domain variables $V(\omega,x), I(\omega,x)$ are replaced by the pair

$$\begin{aligned} \nu_1(\omega,x) &= \frac{1}{2}\left[Z_0^{-\frac{1}{2}}(x)U(\omega,x) - Z_0^{\frac{1}{2}}(x)I(\omega,x)\right] \\ \nu_2(\omega,x) &= \frac{1}{2}\left[Z_0^{-\frac{1}{2}}(x)U(\omega,x) + Z_0^{\frac{1}{2}}(x)I(\omega,x)\right] \end{aligned} \tag{41}$$

with

$$Z_0(x) = \sqrt{\frac{L(x)}{C(x)}}. \tag{42}$$

These transformations lead to the Zakharov-Shabat equations

$$\begin{aligned} \frac{d\nu_1(\omega,x)}{dx} + ik\nu_1(\omega,x) &= q^*(x)\nu_1(\omega,x) + q^+(x)\nu_2(\omega,x) \\ \frac{d\nu_2(\omega,x)}{dx} - ik\nu_2(\omega,x) &= q^-(x)\nu_1(\omega,x) - q^*(x)\nu_2(\omega,x) \end{aligned} \tag{43}$$

with

$$\begin{aligned} q^{\pm}(x) &= -\frac{1}{4}\frac{d}{dx}\left[ln\frac{L(x)}{C(x)}\right] \mp \frac{1}{2}\left[\frac{R(x)}{L(x)} - \frac{G(x)}{C(x)}\right] \\ &= -\frac{1}{2Z_0(x)}\frac{d}{dx}Z_0(x) \mp \frac{1}{2}\left[\frac{R(x)}{L(x)} - \frac{G(x)}{C(x)}\right] \\ q^*(x) &= \frac{1}{2}\left[\frac{R(x)}{L(x)} + \frac{G(x)}{C(x)}\right]. \end{aligned} \tag{44}$$

These equations have been well studied in the inverse scattering theory, for the purpose of determining partly the "potential functions" $q^{\pm}(x)$ and $q^*(x)$ from the scattering data matrix, which turns out to correspond to the data typically collected with reflectometry instruments. For instance, it is possible to compute the function $Z_0(x)$ defined in (36), often known as the characteristic impedance, from the reflection coefficient measured at one end of the cable. Such an example is illustrated in Figure 3 . Any fault affecting the characteristic impedance, like in the example of Figure 3 caused by a slight geometric deformation, can thus be efficiently detected, localized and characterized.

3.4. Research Program

The research will first focus on the extension and implementation of current techniques as developed in I4S and IFSTTAR. Before doing any temperature rejection on large scale structures as planned, we need to develop good and accurate models of thermal fields. We also need to develop robust and efficient versions of our algorithms, mainly the subspace algorithms before envisioning linking them with physical models. Briefly, we need to mature our statistical toolset as well as our physical modeling before mixing them together later on.

3.4.1. Vibration analysis and monitoring

3.4.1.1. Direct vibration modeling under temperature changes

This task builds upon what has been achieved in the CONSTRUCTIF project, where a simple formulation of the temperature effect has been exhibited, based on relatively simple assumptions. The next step is to generalize this modeling to a realistic large structure under complex thermal changes. Practically, temperature and resulting structural prestress and pre strains of thermal origin are not uniform and civil structures are complex. This leads to a fully 3D temperature field, not just a single value. Inertia effects also forbid a trivial prediction of the temperature based on current sensor outputs while ignoring past data. On the other side, the temperature is seen as a nuisance. That implies that any damage detection procedure has first to correct the temperature effect prior to any detection.

Modeling vibrations of structures under thermal prestress does and will play an important role in the static correction of kinematic measurements, in health monitoring methods based on vibration analysis as well as in durability and in the active or semi-active control of civil structures that by nature are operated under changing environmental conditions. As a matter of fact, using temperature and dynamic models the project aims at correcting the current vibration state from induced temperature effects, such that damage detection algorithms rely on a comparison of this thermally corrected current vibration state with a reference state computed or measured at a reference temperature. This approach is expected to cure damage detection algorithms from the environmental variations.

I4S will explore various ways of implementing this concept, notably within the FUI SIPRIS project.

3.4.1.2. Damage localization algorithms (in the case of localized damages such as cracks)

During the CONSTRUCTIF project, both feasibility and efficiency of some damage detection and localization algorithms were proved. Those methods are based on the tight coupling of statistical algorithms with finite element models. It has been shown that effective localization of some damaged elements was possible, and this was validated on a numerical simulated bridge deck model. Still, this approach has to be validated on real structures.

On the other side, new localization algorithms are currently investigated such as the one developed conjointly with University of Boston and tested within the framework of FP7 ISMS project. These algorithms will be implemented and tested on the PEGASE platform as well as all our toolset.

When possible, link with temperature rejection will be done along the lines of what has been achieved in the CONSTRUCTIF project.

3.4.1.3. Uncertainty quantification for system identification algorithms

Some emphasis will be put on expressing confidence intervals for system identification. It is a primary goal to take into account the uncertainty within the identification procedure, using either identification algorithms derivations or damage detection principles. Such algorithms are critical for both civil and aeronautical structures monitoring. It has been shown that confidence intervals for estimation parameters can theoretically be related to the damage detection techniques and should be computed as a function of the Fisher information matrix associated to the damage detection test. Based on those assumptions, it should be possible to obtain confidence intervals for a large class of estimates, from damping to finite elements models. Uncertainty considerations are also deeply investigated in collaboration with Dassault Aviation in Mellinger PhD thesis or with Northeastern University, Boston, within Gallegos PhD thesis.

3.4.2. Reflectometry-based methods for civil engineering structure health monitoring

The inverse scattering method we developed is efficient for the diagnosis of all soft faults affecting the characteristic impedance, the major parameter of a cable. In some particular applications, however, faults would rather affect the series resistance (ohmic loss) or shunt conductance (leakage loss) than the characteristic impedance. The first method we developed for the diagnosis of such losses had some numerical stability problems. The new method [46], [26] is much more reliable and efficient. It is also important to develop efficient solutions for long cables, up to a few kilometers.

For wired networks, the methods we already developed cover either the case of simple networks with a single node measurement or the case of complex networks with complete node measurements. Further developments are still necessary for intermediate situations.

In terms of applications, the use of electric cables as sensors for the monitoring of various structures is still at its beginning. We believe that this new technology has a strong potential in different fields, notably in civil engineering and in materials engineering.

3.4.3. Non Destructive testing of CFRP bonded on concrete through active thermography

Strengthening or retrofitting of reinforced concrete structures by externally bonded fibre-reinforced polymer (FRP) systems is now a commonly accepted and widespread technique. However, the use of bonding techniques always implies following rigorous installation procedures. The number of carbon fibre-reinforced polymer (CFRP) sheets and the glue layer thickness are designed by civil engineers to address strengthening objectives. Moreover, professional crews have to be trained accordingly in order to ensure the durability and long-term performance of the FRP reinforcements. Conformity checking through an ‘in situ’ verification of the bonded FRP systems is then highly desirable. The quality control programme should involve a set of adequate inspections and tests. Visual inspection and acoustic sounding (hammer tap) are commonly used to detect delaminations (disbonds). Nevertheless, these techniques are unable to provide sufficient information about the depth (in case of multilayered composite) and width of the disbonded areas. They are also incapable of evaluating the degree of adhesion between the FRP and the substrate (partial delamination, damage of the resin and poor mechanical properties of the resin). Consequently, rapid and efficient inspection methods are required. Among the non-destructive (NDT) methods currently under study, active infrared thermography is investigated due to its ability to be used in the field. In such context and to reach the aim of having an in situ efficient NDT method, we carried out experiments and subsequent data analysis using thermal excitation. Image processing, inverse thermal modelling and 3D numerical simulations are used and then applied to experimental data obtained in laboratory conditions.

3.4.4. IRSHM: Multi-Sensing system for outdoor thermal monitoring

Ageing of transport infrastructures combined with traffic and climatic solicitations contribute to the reduction of their performances. To address and quantify the resilience of civil engineering structure, investigations on robust, fast and efficient methods are required. Among research works carried out at IFSTTAR, methods for long term monitoring face an increasing demand. Such works take benefits of this last decade technological progresses in ICT domain.

Thanks to IFSTTAR years of experience in large scale civil engineering experiment, I4S is able to perform very long term thermal monitoring of structures exposed to environmental condition, as the solar heat flux, natural convection or seasonal perturbation. Informations system are developed to asses the data acquisition and researchers work on the quantification of the data to detect flaws emergence on structure, those techniques are also used to diagnose thermal insulation of buildings or monitoring of guided transport infrastructures, Figure 4 left. Experiments are carried out on a real transport infrastructure open to traffic and buildings. The detection of the inner structure of the deck is achieved by image processing techniques (as FFT), principal component thermography (PCT), Figure 4 right, or characterization of the inner structure thanks to an original image processing approach.

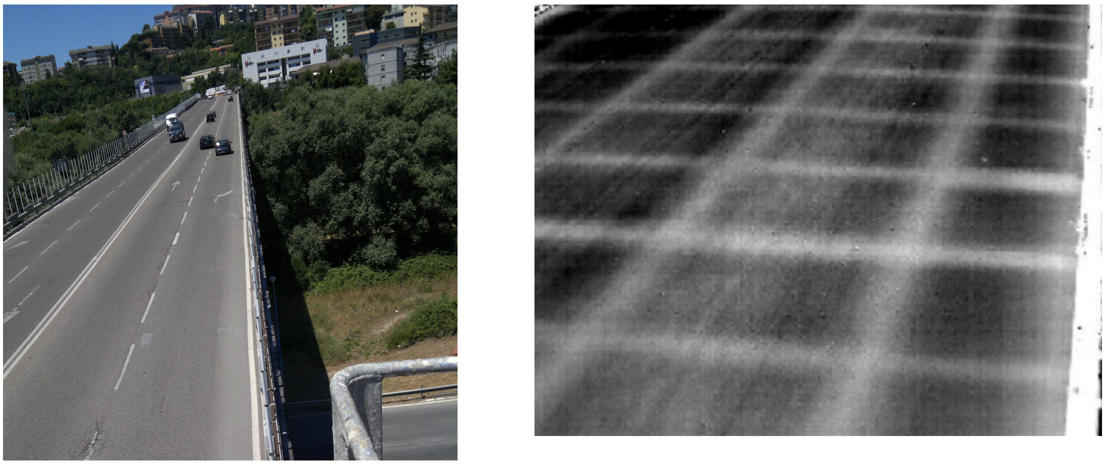


Figure 4. Left: Image in the visible spectrum of the deck surface - Right: PCT result on a bridge deck

For the next few years, I4S is actively implied in the SenseCity EQUIPEX (http://sense-city.ifsttar.fr/) where our informations systems are used to monitor a mini-city replica, Figure 5 .

3.4.5. R5G: The 5th Generation Road

The road has to reinvent itself periodically in response to innovations, societal issues and rising user expectations. The 5th Generation Road (R5G) focuses firmly on the future and sets out to be automated, safe, sustainable and suited to travel needs. Several research teams are involved in work related to this flagship project for IFSTTAR, which is a stakeholder in the Forever Open Road. Through its partnership with the COSYS (IFSTTAR) department, I4S is fully implicated in the development of the 5th Generation Road.

Most of the innovations featured in R5G are now mature, for example communication and few solutions for energy exchange between the infrastructure, the vehicle and the network manager; recyclable materials with the potential for self-diagnosis and repair, a pavement surface that remains permanently optimal irrespective of climatic variations… Nevertheless, implementing them on an industrial scale at a reasonable cost still represents a real challenge. Consultation with the stakeholders (researchers, industry, road network owners

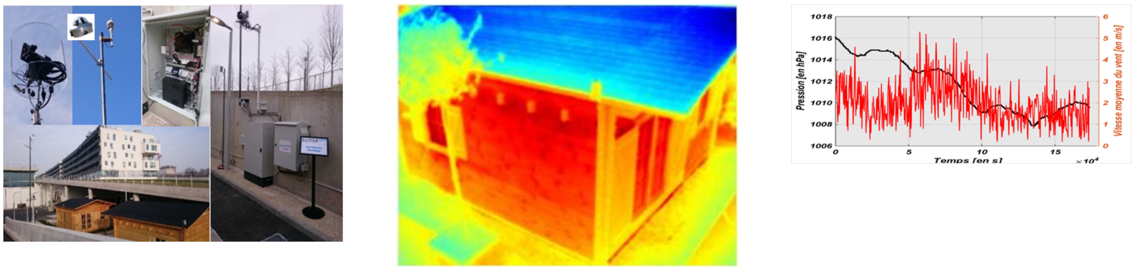


Figure 5. Various view and results of the SenseCity experimentation site - (site and hardware view, IR imaging, Environmental Monitoring)

and users) has already established the priorities for the creation of full-scale demonstrators. The next stages are to achieve synergy between the technologies tested by the demonstrators, to manage the interfaces and get society to adopt R5G.

INOCS Team

3. Research Program

3.1. Introduction

An optimization problem consists in finding a best solution from a set of feasible solutions. Such a problem can be typically modeled as a mathematical program in which decision variables must

1. satisfy a set of constraints that translate the feasibility of the solution and
2. optimize some (or several) objective function(s). Optimization problems are usually classified according to types of decision to be taken into strategic, tactical and operational problems.

We consider that an optimization problem presents a complex structure when it involves decisions of different types/nature (i.e. strategic, tactical or operational), and/or presenting some hierarchical leader-follower structure. The set of constraints may usually be partitioned into global constraints linking variables associated with the different types/nature of decision and constraints involving each type of variables separately. Optimization problems with a complex structure lead to extremely challenging problems since a global optimum with respect to the whole sets of decision variables and of constraints must be determined.

Significant progresses have been made in optimization to solve academic problems. Nowadays large-scale instances of some NP-Hard problems are routinely solved to optimality. *Our vision within INOCS is to make the same advances while addressing CS optimization problems*. To achieve this goal we aim to develop global solution approaches at the opposite of the current trend. INOCS team members have already proposed some successful methods following this research lines to model and solve CS problems (e.g. ANR project RESPET, Brotcorne *et al.* 2011, 2012, Gendron *et al.* 2009, Strack *et al.* 2009). However, these are preliminary attempts and a number of challenges regarding modeling and methodological issues have still to be met.

3.2. Modeling problems with complex structures

A classical optimization problem can be formulated as follows:

$$\begin{array}{ll} \min & f(x) \\ s.t. & x \in X, \end{array} \tag{45}$$

In this problem, X is the set of feasible solutions. Typically, in mathematical programming, X is defined by a set of constraints. x may be also limited to non-negative integer values.

INOCS team plan to address optimization problem where two types of decision are addressed jointly and are interrelated. More precisely, let us assume that variables x and y are associated with these decisions. A generic model for CS problems is the following:

$$\begin{array}{ll} \min & g(x,y) \\ s.t. & x \in X, \\ (x,y) & \in XY, \\ y & \in Y(x). \end{array} \tag{46}$$

In this model, X is the set of feasible values for x. XY is the set of feasible values for x and y jointly. This set is typically modeled through linking constraints. Last, $Y(x)$ is the set of feasible values for y for a given x. In INOCS, we do not assume that $Y(x)$ has any properties.

The INOCS team plans to model optimization CS problems according to three types of optimization paradigms: large scale complex structures optimization, bilevel optimization and robust/stochastic optimization. These paradigms instantiate specific variants of the generic model.

Large scale complex structures optimization problems can be formulated through the simplest variant of the generic model given above. In this case, it is assumed that $Y(x)$ does not depend on x. In such models, X and Y are associated with constraints on x and on y, XY are the linking constraints. x and y can take continuous or integer values. Note that all the problem data are deterministically known.

Bilevel programs allow the modeling of situations in which a decision-maker, hereafter the leader, optimizes his objective by taking explicitly into account the response of another decision maker or set of decision makers (the follower) to his/her decisions. Bilevel programs are closely related to Stackelberg (leader-follower) games as well as to the principal-agent paradigm in economics. In other words, bilevel programs can be considered as demand-offer equilibrium models where the demand is the result of another mathematical problem. Bilevel problems can be formulated through the generic CS model when $Y(x)$ corresponds to the optimal solutions of a mathematical program defined for a given x, i.e. $Y(x) = \operatorname{argmin} \{h(x,y)|y \in Y_2, (x,y) \in XY_2\}$ where Y_2 is defined by a set of constraints on y, and XY_2 is associated with the linking constraints.

In robust/stochastic optimization, it is assumed that the data related to a problem are subject to uncertainty. In stochastic optimization, probability distributions governing the data are known, and the objective function involves mathematical expectation(s). In robust optimization, uncertain data take value within specified sets, and the function to optimize is formulated in terms of a min-max objective typically (the solution must be optimal for the worst-case scenario). . A standard modeling of uncertainty on data is obtained by defining a set of possible scenarios that can be described explicitly or implicitly. In stochastic optimization, in addition, a probability of occurrence is associated with each scenario and the expected objective value is optimized.

3.3. Solving problems with complex structures

Standard solution methods developed for CS problems solve independent sub-problems associated with each type of variables without explicitly integrating their interactions or integrating them iteratively in a heuristic way. However these subproblems are intrinsically linked and should be addressed jointly. In *mathematicaloptimization* a classical approach is to approximate the convex hull of the integer solutions of the model by its linear relaxation. The main solution methods are i) polyhedral solution methods which strengthen this linear relaxation by adding valid inequalities, ii) decomposition solution methods (Dantzig Wolfe, Lagrangian Relaxation, Benders decomposition) which aim to obtain a better approximation and solve it by generating extreme points/rays. Main challenges are i) the analysis of the strength of the cuts and their separations for polyhedral solution methods, ii) the decomposition schemes and iii) the extreme points/rays generations for the decomposition solution methods.

The main difficulty in solving *bilevel problems* is due to their non convexity and non differentiability. Even linear bilevel programs, where all functions involved are affine, are computationally challenging despite their apparent simplicity . Up to now, much research has been devoted to bilevel problems with linear or convex follower problems. In this case, the problem can be reformulated as a single-level program involving complementarity constraints, exemplifying the dual nature, continuous and combinatorial, of bilevel programs.

IPSO Project-Team

3. Research Program

3.1. Structure-preserving numerical schemes for solving ordinary differential equations

Participants: François Castella, Philippe Chartier, Erwan Faou.

ordinary differential equation, numerical integrator, invariant, Hamiltonian system, reversible system, Lie-group system

In many physical situations, the time-evolution of certain quantities may be written as a Cauchy problem for a differential equation of the form

$$\begin{aligned} y'(t) &= f(y(t)), \\ y(0) &= y_0. \end{aligned} \tag{47}$$

For a given y_0, the solution $y(t)$ at time t is denoted $\varphi_t(y_0)$. For fixed t, φ_t becomes a function of y_0 called the *flow* of (1). From this point of view, a numerical scheme with step size h for solving (1) may be regarded as an approximation Φ_h of φ_h. One of the main questions of *geometric integration* is whether *intrinsic* properties of φ_t may be passed on to Φ_h.

This question can be more specifically addressed in the following situations:

3.1.1. Reversible ODEs

The system (1) is said to be ρ-reversible if there exists an involutive linear map ρ such that

$$\rho \circ \varphi_t = \varphi_t^{-1} \circ \rho = \varphi_{-t} \circ \rho. \tag{48}$$

It is then natural to require that Φ_h satisfies the same relation. If this is so, Φ_h is said to be *symmetric*. Symmetric methods for reversible systems of ODEs are just as much important as *symplectic* methods for Hamiltonian systems and offer an interesting alternative to symplectic methods.

3.1.2. ODEs with an invariant manifold

The system (1) is said to have an invariant manifold g whenever

$$\mathcal{M} = \{y \in \mathbb{R}^n; g(y) = 0\} \tag{49}$$

is kept *globally* invariant by φ_t. In terms of derivatives and for sufficiently differentiable functions f and g, this means that

$$\forall\, y \in \mathcal{M},\ g'(y)f(y) = 0.$$

As an example, we mention Lie-group equations, for which the manifold has an additional group structure. This could possibly be exploited for the space-discretisation. Numerical methods amenable to this sort of problems have been reviewed in a recent paper [48] and divided into two classes, according to whether they use g explicitly or through a projection step. In both cases, the numerical solution is forced to live on the manifold at the expense of some Newton's iterations.

3.1.3. Hamiltonian systems

Hamiltonian problems are ordinary differential equations of the form:

$$\begin{array}{rcrcl} \dot{p}(t) & = & -\nabla_q H(p(t),q(t)) & \in & \mathbb{R}^d \\ \dot{q}(t) & = & \nabla_p H(p(t),q(t)) & \in & \mathbb{R}^d \end{array} \tag{50}$$

with some prescribed initial values $(p(0),q(0)) = (p_0,q_0)$ and for some scalar function H, called the Hamiltonian. In this situation, H is an invariant of the problem. The evolution equation (4) can thus be regarded as a differential equation on the manifold

$$\mathcal{M} = \{(p,q) \in \mathbb{R}^d \times \mathbb{R}^d; H(p,q) = H(p_0,q_0)\}.$$

Besides the Hamiltonian function, there might exist other invariants for such systems: when there exist d invariants in involution, the system (4) is said to be *integrable*. Consider now the parallelogram P originating from the point $(p,q) \in \mathbb{R}^{2d}$ and spanned by the two vectors $\xi \in \mathbb{R}^{2d}$ and $\eta \in \mathbb{R}^{2d}$, and let $\omega(\xi,\eta)$ be the sum of the *oriented* areas of the projections over the planes (p_i,q_i) of P,

$$\omega(\xi,\eta) = \xi^T J \eta,$$

where J is the *canonical symplectic* matrix

$$J = \left[\begin{array}{cc} 0 & I_d \\ -I_d & 0 \end{array} \right].$$

A continuously differentiable map g from $\mathbb{R}^{2d}$ to itself is called symplectic if it preserves ω, i.e. if

$$\omega(g'(p,q)\xi, g'(p,q)\eta) = \omega(\xi,\eta).$$

A fundamental property of Hamiltonian systems is that their exact flow is symplectic. Integrable Hamiltonian systems behave in a very remarkable way: as a matter of fact, their invariants persist under small perturbations, as shown in the celebrated theory of Kolmogorov, Arnold and Moser. This behavior motivates the introduction of *symplectic* numerical flows that share most of the properties of the exact flow. For practical simulations of Hamiltonian systems, symplectic methods possess an important advantage: the error-growth as a function of time is indeed linear, whereas it would typically be quadratic for non-symplectic methods.

3.1.4. Differential-algebraic equations

Whenever the number of differential equations is insufficient to determine the solution of the system, it may become necessary to solve the differential part and the constraint part altogether. Systems of this sort are called differential-algebraic systems. They can be classified according to their index, yet for the purpose of this expository section, it is enough to present the so-called index-2 systems

$$\begin{array}{rcl} \dot{y}(t) & = & f(y(t), z(t)), \\ 0 & = & g(y(t)), \end{array} \tag{51}$$

where initial values $(y(0), z(0)) = (y_0, z_0)$ are given and assumed to be consistent with the constraint manifold. By constraint manifold, we imply the intersection of the manifold

$$\mathcal{M}_1 = \{y \in \mathbb{R}^n, g(y) = 0\}$$

and of the so-called hidden manifold

$$\mathcal{M}_2 = \{(y,z) \in \mathbb{R}^n \times \mathbb{R}^m, \frac{\partial g}{\partial y}(y) f(y,z) = 0\}.$$

This manifold $\mathcal{M} = \mathcal{M}_1 \bigcap \mathcal{M}_2$ is the manifold on which the exact solution $(y(t), z(t))$ of (5) lives.

There exists a whole set of schemes which provide a numerical approximation lying on $\mathcal{M}_1$. Furthermore, this solution can be projected on the manifold $\mathcal{M}$ by standard projection techniques. However, it it worth mentioning that a projection destroys the symmetry of the underlying scheme, so that the construction of a symmetric numerical scheme preserving $\mathcal{M}$ requires a more sophisticated approach.

3.2. Highly-oscillatory systems

Participants: François Castella, Philippe Chartier, Nicolas Crouseilles, Erwan Faou, Florian Méhats, Mohammed Lemou.

second-order ODEs, oscillatory solutions, Schrödinger and wave equations, step size restrictions.

In applications to molecular dynamics or quantum dynamics for instance, the right-hand side of (1) involves *fast* forces (short-range interactions) and *slow* forces (long-range interactions). Since *fast* forces are much cheaper to evaluate than *slow* forces, it seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

A typical model of highly-oscillatory systems is the second-order differential equations

$$\ddot{q} \quad = \quad -\nabla V(q) \tag{52}$$

where the potential $V(q)$ is a sum of potentials $V = W + U$ acting on different time-scales, with $\nabla^2 W$ positive definite and $\|\nabla^2 W\| >> \|\nabla^2 U\|$. In order to get a bounded error propagation in the linearized equations for an explicit numerical method, the step size must be restricted according to

$$h\omega < C,$$

where C is a constant depending on the numerical method and where ω is the highest frequency of the problem, i.e. in this situation the square root of the largest eigenvalue of $\nabla^2 W$. In applications to molecular dynamics for instance, *fast* forces deriving from W (short-range interactions) are much cheaper to evaluate than *slow* forces deriving from U (long-range interactions). In this case, it thus seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

Another prominent example of highly-oscillatory systems is encountered in quantum dynamics where the Schrödinger equation is the model to be used. Assuming that the Laplacian has been discretized in space, one indeed gets the *time*-dependent Schrödinger equation:

$$i\dot{\psi}(t) = \frac{1}{\varepsilon} H(t) \psi(t), \tag{53}$$

where $H(t)$ is finite-dimensional matrix and where ε typically is the square-root of a mass-ratio (say electron/ion for instance) and is small ($\varepsilon \approx 10^{-2}$ or smaller). Through the coupling with classical mechanics ($H(t)$ is obtained by solving some equations from classical mechanics), we are faced once again with two different time-scales, 1 and ε. In this situation also, it is thus desirable to devise a numerical method able to advance the solution by a time-step $h > \varepsilon$.

3.3. Geometric schemes for the Schrödinger equation

Participants: François Castella, Philippe Chartier, Erwan Faou, Florian Méhats.

Schrödinger equation, variational splitting, energy conservation.

Given the Hamiltonian structure of the Schrödinger equation, we are led to consider the question of energy preservation for time-discretization schemes.

At a higher level, the Schrödinger equation is a partial differential equation which may exhibit Hamiltonian structures. This is the case of the time-dependent Schrödinger equation, which we may write as

$$i\varepsilon\frac{\partial\psi}{\partial t} = H\psi, \tag{54}$$

where $\psi = \psi(x,t)$ is the wave function depending on the spatial variables $x = (x_1, \cdots, x_N)$ with $x_k \in \mathbb{R}^d$ (e.g., with $d = 1$ or 3 in the partition) and the time $t \in \mathbb{R}$. Here, ε is a (small) positive number representing the scaled Planck constant and i is the complex imaginary unit. The Hamiltonian operator H is written

$$H = T + V$$

with the kinetic and potential energy operators

$$T = -\sum_{k=1}^{N}\frac{\varepsilon^2}{2m_k}\Delta_{x_k} \quad \text{and} \quad V = V(x),$$

where $m_k > 0$ is a particle mass and Δ_{x_k} the Laplacian in the variable $x_k \in \mathbb{R}^d$, and where the real-valued potential V acts as a multiplication operator on ψ.

The multiplication by i in (8) plays the role of the multiplication by J in classical mechanics, and the energy $\langle\psi|H|\psi\rangle$ is conserved along the solution of (8), using the physicists' notations $\langle u|A|u\rangle = \langle u, Au\rangle$ where $\langle\ ,\ \rangle$ denotes the Hermitian L^2-product over the phase space. In quantum mechanics, the number N of particles is very large making the direct approximation of (8) very difficult.

The numerical approximation of (8) can be obtained using projections onto submanifolds of the phase space, leading to various PDEs or ODEs: see [52], [51] for reviews. However the long-time behavior of these approximated solutions is well understood only in this latter case, where the dynamics turns out to be finite dimensional. In the general case, it is very difficult to prove the preservation of qualitative properties of (8) such as energy conservation or growth in time of Sobolev norms. The reason for this is that backward error analysis is not directly applicable for PDEs. Overwhelming these difficulties is thus a very interesting challenge.

A particularly interesting case of study is given by symmetric splitting methods, such as the Strang splitting:

$$\psi_1 = \exp\left(-i(\delta t)V/2\right)\exp\left(i(\delta t)\Delta\right)\exp\left(-i(\delta t)V/2\right)\psi_0 \tag{55}$$

where δt is the time increment (we have set all the parameters to 1 in the equation). As the Laplace operator is unbounded, we cannot apply the standard methods used in ODEs to derive long-time properties of these schemes. However, its projection onto finite dimensional submanifolds (such as Gaussian wave packets space or FEM finite dimensional space of functions in x) may exhibit Hamiltonian or Poisson structure, whose long-time properties turn out to be more tractable.

3.4. High-frequency limit of the Helmholtz equation

Participant: François Castella.

waves, Helmholtz equation, high oscillations.

The Helmholtz equation models the propagation of waves in a medium with variable refraction index. It is a simplified version of the Maxwell system for electro-magnetic waves.

The high-frequency regime is characterized by the fact that the typical wavelength of the signals under consideration is much smaller than the typical distance of observation of those signals. Hence, in the high-frequency regime, the Helmholtz equation at once involves highly oscillatory phenomena that are to be described in some asymptotic way. Quantitatively, the Helmholtz equation reads

$$i\alpha_\varepsilon u_\varepsilon(x) + \varepsilon^2 \Delta_x u_\varepsilon + n^2(x) u_\varepsilon = f_\varepsilon(x). \tag{56}$$

Here, ε is the small adimensional parameter that measures the typical wavelength of the signal, $n(x)$ is the space-dependent refraction index, and $f_\varepsilon(x)$ is a given (possibly dependent on ε) source term. The unknown is $u_\varepsilon(x)$. One may think of an antenna emitting waves in the whole space (this is the $f_\varepsilon(x)$), thus creating at any point x the signal $u_\varepsilon(x)$ along the propagation. The small $\alpha_\varepsilon > 0$ term takes into account damping of the waves as they propagate.

One important scientific objective typically is to describe the high-frequency regime in terms of *rays* propagating in the medium, that are possibly refracted at interfaces, or bounce on boundaries, etc. Ultimately, one would like to replace the true numerical resolution of the Helmholtz equation by that of a simpler, asymptotic model, formulated in terms of rays.

In some sense, and in comparison with, say, the wave equation, the specificity of the Helmholtz equation is the following. While the wave equation typically describes the evolution of waves between some initial time and some given observation time, the Helmholtz equation takes into account at once the propagation of waves over *infinitely long* time intervals. Qualitatively, in order to have a good understanding of the signal observed in some bounded region of space, one readily needs to be able to describe the propagative phenomena in the whole space, up to infinity. In other words, the “rays” we refer to above need to be understood from the initial time up to infinity. This is a central difficulty in the analysis of the high-frequency behaviour of the Helmholtz equation.

3.5. From the Schrödinger equation to Boltzmann-like equations

Participant: François Castella.

Schrödinger equation, asymptotic model, Boltzmann equation.

The Schrödinger equation is the appropriate way to describe transport phenomena at the scale of electrons. However, for real devices, it is important to derive models valid at a larger scale.

In semi-conductors, the Schrödinger equation is the ultimate model that allows to obtain quantitative information about electronic transport in crystals. It reads, in convenient adimensional units,

$$i\partial_t \psi(t,x) = -\frac{1}{2}\Delta_x \psi + V(x)\psi, \tag{57}$$

where $V(x)$ is the potential and $\psi(t,x)$ is the time- and space-dependent wave function. However, the size of real devices makes it important to derive simplified models that are valid at a larger scale. Typically, one wishes to have kinetic transport equations. As is well-known, this requirement needs one to be able to describe “collisions” between electrons in these devices, a concept that makes sense at the macroscopic level, while it does not at the microscopic (electronic) level. Quantitatively, the question is the following: can one obtain the Boltzmann equation (an equation that describes collisional phenomena) as an asymptotic model for the Schrödinger equation, along the physically relevant micro-macro asymptotics? From the point of view of modelling, one wishes here to understand what are the “good objects”, or, in more technical words, what are the relevant “cross-sections”, that describe the elementary collisional phenomena. Quantitatively, the Boltzmann equation reads, in a simplified, linearized, form :

$$\partial_t f(t,x,v) = \int_{\mathbf{R}^3} \sigma(v,v')\ [f(t,x,v') - f(t,x,v)]dv'. \tag{58}$$

Here, the unknown is $f(x,v,t)$, the probability that a particle sits at position x, with a velocity v, at time t. Also, $\sigma(v,v')$ is called the cross-section, and it describes the probability that a particle “jumps” from velocity v to velocity v' (or the converse) after a collision process.

MATHERIALS Project-Team

3. Research Program

3.1. Research Program

Quantum Chemistry aims at understanding the properties of matter through the modelling of its behavior at a subatomic scale, where matter is described as an assembly of nuclei and electrons. At this scale, the equation that rules the interactions between these constitutive elements is the Schrödinger equation. It can be considered (except in few special cases notably those involving relativistic phenomena or nuclear reactions) as a universal model for at least three reasons. First it contains all the physical information of the system under consideration so that any of the properties of this system can in theory be deduced from the Schrödinger equation associated to it. Second, the Schrödinger equation does not involve any empirical parameters, except some fundamental constants of Physics (the Planck constant, the mass and charge of the electron, ...); it can thus be written for any kind of molecular system provided its chemical composition, in terms of natures of nuclei and number of electrons, is known. Third, this model enjoys remarkable predictive capabilities, as confirmed by comparisons with a large amount of experimental data of various types. On the other hand, using this high quality model requires working with space and time scales which are both very tiny: the typical size of the electronic cloud of an isolated atom is the Angström (10^{-10} meters), and the size of the nucleus embedded in it is 10^{-15} meters; the typical vibration period of a molecular bond is the femtosecond (10^{-15} seconds), and the characteristic relaxation time for an electron is 10^{-18} seconds. Consequently, Quantum Chemistry calculations concern very short time (say 10^{-12} seconds) behaviors of very small size (say 10^{-27} m^3) systems. The underlying question is therefore whether information on phenomena at these scales is useful in understanding or, better, predicting macroscopic properties of matter. It is certainly not true that *all* macroscopic properties can be simply upscaled from the consideration of the short time behavior of a tiny sample of matter. Many of them derive from ensemble or bulk effects, that are far from being easy to understand and to model. Striking examples are found in solid state materials or biological systems. Cleavage, the ability of minerals to naturally split along crystal surfaces (e.g. mica yields to thin flakes), is an ensemble effect. Protein folding is also an ensemble effect that originates from the presence of the surrounding medium; it is responsible for peculiar properties (e.g. unexpected acidity of some reactive site enhanced by special interactions) upon which vital processes are based. However, it is undoubtedly true that *many* macroscopic phenomena originate from elementary processes which take place at the atomic scale. Let us mention for instance the fact that the elastic constants of a perfect crystal or the color of a chemical compound (which is related to the wavelengths absorbed or emitted during optic transitions between electronic levels) can be evaluated by atomic scale calculations. In the same fashion, the lubricative properties of graphite are essentially due to a phenomenon which can be entirely modeled at the atomic scale. It is therefore reasonable to simulate the behavior of matter at the atomic scale in order to understand what is going on at the macroscopic one. The journey is however a long one. Starting from the basic principles of Quantum Mechanics to model the matter at the subatomic scale, one finally uses statistical mechanics to reach the macroscopic scale. It is often necessary to rely on intermediate steps to deal with phenomena which take place on various *mesoscales*. It may then be possible to couple one description of the system with some others within the so-called *multiscale* models. The sequel indicates how this journey can be completed focusing on the first smallest scales (the subatomic one), rather than on the larger ones. It has already been mentioned that at the subatomic scale, the behavior of nuclei and electrons is governed by the Schrödinger equation, either in its time-dependent form or in its time-independent form. Let us only mention at this point that

- both equations involve the quantum Hamiltonian of the molecular system under consideration; from a mathematical viewpoint, it is a self-adjoint operator on some Hilbert space; *both* the Hilbert space and the Hamiltonian operator depend on the nature of the system;
- also present into these equations is the wavefunction of the system; it completely describes its state; its L^2 norm is set to one.

The time-dependent equation is a first-order linear evolution equation, whereas the time-independent equation is a linear eigenvalue equation. For the reader more familiar with numerical analysis than with quantum mechanics, the linear nature of the problems stated above may look auspicious. What makes the numerical simulation of these equations extremely difficult is essentially the huge size of the Hilbert space: indeed, this space is roughly some symmetry-constrained subspace of $L^2(\mathbb{R}^d)$, with $d = 3(M + N)$, M and N respectively denoting the number of nuclei and the number of electrons the system is made of. The parameter d is already 39 for a single water molecule and rapidly reaches 10^6 for polymers or biological molecules. In addition, a consequence of the universality of the model is that one has to deal at the same time with several energy scales. In molecular systems, the basic elementary interaction between nuclei and electrons (the two-body Coulomb interaction) appears in various complex physical and chemical phenomena whose characteristic energies cover several orders of magnitude: the binding energy of core electrons in heavy atoms is 10^4 times as large as a typical covalent bond energy, which is itself around 20 times as large as the energy of a hydrogen bond. High precision or at least controlled error cancellations are thus required to reach chemical accuracy when starting from the Schrödinger equation. Clever approximations of the Schrödinger problems are therefore needed. The main two approximation strategies, namely the Born-Oppenheimer-Hartree-Fock and the Born-Oppenheimer-Kohn-Sham strategies, end up with large systems of coupled *nonlinear* partial differential equations, each of these equations being posed on $L^2(\mathbb{R}^3)$. The size of the underlying functional space is thus reduced at the cost of a dramatic increase of the mathematical complexity of the problem: nonlinearity. The mathematical and numerical analysis of the resulting models has been the major concern of the project-team for a long time. In the recent years, while part of the activity still follows this path, the focus has progressively shifted to problems at other scales. Such problems are described in the following sections.

MATHRISK Project-Team

3. Research Program

3.1. Dependence modeling

Participants: Aurélien Alfonsi, Benjamin Jourdain, Damien Lamberton, Bernard Lapeyre.

The volatility is a key concept in modern mathematical finance, and an indicator of the market stability. Risk management and associated instruments depend strongly on the volatility, and volatility modeling has thus become a crucial issue in the finance industry. Of particular importance is the assets *dependence* modeling. The calibration of models for a single asset can now be well managed by banks but modeling of dependence is the bottleneck to efficiently aggregate such models. A typical issue is how to go from the individual evolution of each stock belonging to an index to the joint modeling of these stocks. In this perspective, we want to model stochastic volatility in a *multidimensional* framework. To handle these questions mathematically, we have to deal with stochastic differential equations that are defined on matrices in order to model either the instantaneous covariance or the instantaneous correlation between the assets. From a numerical point of view, such models are very demanding since the main indexes include generally more than thirty assets. It is therefore necessary to develop efficient numerical methods for pricing options and calibrating such models to market data. As a first application, modeling the dependence between assets allows us to better handle derivatives products on a basket. It would give also a way to price and hedge consistenly single-asset and basket products. Besides, it can be a way to capture how the market estimates the dependence between assets. This could give some insights on how the market anticipates the systemic risk.

3.2. Liquidity risk

Participants: Aurélien Alfonsi, Agnès Bialobroda Sulem, Antonino Zanette.

The financial crisis has caused an increased interest in mathematical finance studies which take into account the market incompleteness issue and the liquidity risk. Loosely speaking, liquidity risk is the risk that comes from the difficulty of selling (or buying) an asset. At the extreme, this may be the impossibility to sell an asset, which occurred for "junk assets" during the subprime crisis. Hopefully, it is in general possible to sell assets, but this may have some cost. Let us be more precise. Usually, assets are quoted on a market with a Limit Order Book (LOB) that registers all the waiting limit buy and sell orders for this asset. The bid (resp. ask) price is the most expensive (resp. cheapest) waiting buy or sell order. If a trader wants to sell a single asset, he will sell it at the bid price. Instead, if he wants to sell a large quantity of assets, he will have to sell them at a lower price in order to match further waiting buy orders. This creates an extra cost, and raises important issues. From a short-term perspective (from few minutes to some days), this may be interesting to split the selling order and to focus on finding optimal selling strategies. This requires to model the market microstructure, i.e. how the market reacts in a short time-scale to execution orders. From a long-term perspective (typically, one month or more), one has to understand how this cost modifies portfolio managing strategies (especially delta-hedging or optimal investment strategies). At this time-scale, there is no need to model precisely the market microstructure, but one has to specify how the liquidity costs aggregate.

3.2.1. Long term liquidity risk.

On a long-term perspective, illiquidity can be approached via various ways: transactions costs [57], [58], [64], [71], [74], [89], [85], delay in the execution of the trading orders [90], [88], [67], trading constraints or restriction on the observation times (see e.g. [73] and references herein). As far as derivative products are concerned, one has to understand how delta-hedging strategies have to be modified. This has been considered for example by Cetin, Jarrow and Protter [87]. We plan to contribute on these various aspects of liquidity risk modeling and associated stochastic optimization problems. Let us mention here that the price impact generated by the trades of the investor is often neglected with a long-term perspective. This seems acceptable since the investor has time enough to trade slowly in order to eliminate its market impact. Instead, when the investor wants to make significant trades on a very short time horizon, it is crucial to take into account and to model how prices are modified by these trades. This question is addressed in the next paragraph on market microstructure.

3.2.2. Market microstructure.

The European directive MIFID has increased the competition between markets (NYSE-Euronext, Nasdaq, LSE and new competitors). As a consequence, the cost of posting buy or sell orders on markets has decreased, which has stimulated the growth of market makers. Market makers are posting simultaneously bid and ask orders on a same stock, and their profit comes from the bid-ask spread. Basically, their strategy is a "round-trip" (i.e. their position is unchanged between the beginning and the end of the day) that has generated a positive cash flow.

These new rules have also greatly stimulated research on market microstructure modeling. From a practitioner point of view, the main issue is to solve the so-called "optimal execution problem": given a deadline T, what is the optimal strategy to buy (or sell) a given amount of shares that achieves the minimal expected cost? For large amounts, it may be optimal to split the order into smaller ones. This is of course a crucial issue for brokers, but also market makers that are looking for the optimal round-trip.

Solving the optimal execution problem is not only an interesting mathematical challenge. It is also a mean to better understand market viability, high frequency arbitrage strategies and consequences of the competition between markets. For example when modeling the market microstructure, one would like to find conditions that allow or exclude round trips. Beyond this, even if round trips are excluded, it can happen that an optimal selling strategy is made with large intermediate buy trades, which is unlikely and may lead to market instability.

We are interested in finding synthetic market models in which we can describe and solve the optimal execution problem. A. Alfonsi and A. Schied (Mannheim University) [59] have already proposed a simple Limit Order Book model (LOB) in which an explicit solution can be found for the optimal execution problem. We are now interested in considering more sophisticated models that take into account realistic features of the market such as short memory or stochastic LOB. This is mid term objective. At a long term perspective one would like to bridge these models to the different agent behaviors, in order to understand the effect of the different quotation mechanisms (transaction costs for limit orders, tick size, etc.) on the market stability.

3.3. Contagion modeling and systemic risk

Participants: Benjamin Jourdain, Agnès Bialobroda Sulem.

After the recent financial crisis, systemic risk has emerged as one of the major research topics in mathematical finance. The scope is to understand and model how the bankruptcy of a bank (or a large company) may or not induce other bankruptcies. By contrast with the traditional approach in risk management, the focus is no longer on modeling the risks faced by a single financial institution, but on modeling the complex interrelations between financial institutions and the mechanisms of distress propagation among these. Ideally, one would like to be able to find capital requirements (such as the one proposed by the Basel committee) that ensure that the probability of multiple defaults is below some level.

The mathematical modeling of default contagion, by which an economic shock causing initial losses and default of a few institutions is amplified due to complex linkages, leading to large scale defaults, can be addressed by various techniques, such as network approaches (see in particular R. Cont et al. [60] and A. Minca [79]) or mean field interaction models (Garnier-Papanicolaou-Yang [72]). The recent approach in [60] seems very promising. It describes the financial network approach as a weighted directed graph, in which nodes represent financial institutions and edges the exposures between them. Distress propagation in a financial system may be modeled as an epidemics on this graph. In the case of incomplete information on the structure of the interbank network, cascade dynamics may be reduced to the evolution of a multi-dimensional Markov chain that corresponds to a sequential discovery of exposures and determines at any time the size of contagion. Little has been done so far on the *control* of such systems in order to reduce the systemic risk and we aim to contribute to this domain.

3.4. Stochastic analysis and numerical probability

3.4.1. Stochastic control

Participants: Vlad Bally, Jean-Philippe Chancelier, Marie-Claire Quenez, Agnès Bialobroda Sulem.

The financial crisis has caused an increased interest in mathematical finance studies which take into account the market incompleteness issue and the default risk modeling, the interplay between information and performance, the model uncertainty and the associated robustness questions, and various nonlinearities. We address these questions by further developing the theory of stochastic control in a broad sense, including stochastic optimization, nonlinear expectations, Malliavin calculus, stochastic differential games and various aspects of optimal stopping.

3.4.2. Optimal stopping

Participants: Aurélien Alfonsi, Benjamin Jourdain, Damien Lamberton, Agnès Bialobroda Sulem, Marie-Claire Quenez.

The theory of American option pricing has been an incite for a number of research articles about optimal stopping. Our recent contributions in this field concern optimal stopping in models with jumps, irregular obstacles, free boundary analysis, reflected BSDEs.

3.4.3. Simulation of stochastic differential equations

Participants: Benjamin Jourdain, Aurélien Alfonsi, Vlad Bally, Damien Lamberton, Bernard Lapeyre, Jérôme Lelong, Céline Labart.

Effective numerical methods are crucial in the pricing and hedging of derivative securities. The need for more complex models leads to stochastic differential equations which cannot be solved explicitly, and the development of discretization techniques is essential in the treatment of these models. The project MathRisk addresses fundamental mathematical questions as well as numerical issues in the following (non exhaustive) list of topics: Multidimensional stochastic differential equations, High order discretization schemes, Singular stochastic differential equations, Backward stochastic differential equations.

3.4.4. Monte-Carlo simulations

Participants: Benjamin Jourdain, Aurélien Alfonsi, Damien Lamberton, Vlad Bally, Bernard Lapeyre, Ahmed Kebaier, Céline Labart, Jérôme Lelong, Antonino Zanette.

Monte-Carlo methods is a very useful tool to evaluate prices especially for complex models or options. We carry on research on *adaptive variance reduction methods* and to use *Monte-Carlo methods for calibration* of advanced models.

This activity in the MathRisk team is strongly related to the development of the Premia software.

3.4.5. Malliavin calculus and applications in finance

Participants: Vlad Bally, Arturo Kohatsu-Higa, Agnès Bialobroda Sulem, Antonino Zanette.

The original Stochastic Calculus of Variations, now called the Malliavin calculus, was developed by Paul Malliavin in 1976 [77]. It was originally designed to study the smoothness of the densities of solutions of stochastic differential equations. One of its striking features is that it provides a probabilistic proof of the celebrated Hörmander theorem, which gives a condition for a partial differential operator to be hypoelliptic. This illustrates the power of this calculus. In the following years a lot of probabilists worked on this topic and the theory was developed further either as analysis on the Wiener space or in a white noise setting. Many applications in the field of stochastic calculus followed. Several monographs and lecture notes (for example D. Nualart [80], D. Bell [63] D. Ocone [82], B. Øksendal [91]) give expositions of the subject. See also V. Bally [61] for an introduction to Malliavin calculus.

From the beginning of the nineties, applications of the Malliavin calculus in finance have appeared : In 1991 Karatzas and Ocone showed how the Malliavin calculus, as further developed by Ocone and others, could be used in the computation of hedging portfolios in complete markets [81].

Since then, the Malliavin calculus has raised increasing interest and subsequently many other applications to finance have been found [78], such as minimal variance hedging and Monte Carlo methods for option pricing. More recently, the Malliavin calculus has also become a useful tool for studying insider trading models and some extended market models driven by Lévy processes or fractional Brownian motion.

We give below an idea why Malliavin calculus may be a useful instrument for probabilistic numerical methods.

We recall that the theory is based on an integration by parts formula of the form $E(f'(X)) = E(f(X)Q)$. Here X is a random variable which is supposed to be "smooth" in a certain sense and non-degenerated. A basic example is to take $X = \sigma\Delta$ where Δ is a standard normally distributed random variable and σ is a strictly positive number. Note that an integration by parts formula may be obtained just by using the usual integration by parts in the presence of the Gaussian density. But we may go further and take X to be an aggregate of Gaussian random variables (think for example of the Euler scheme for a diffusion process) or the limit of such simple functionals.

An important feature is that one has a relatively explicit expression for the weight Q which appears in the integration by parts formula, and this expression is given in terms of some Malliavin-derivative operators.

Let us now look at one of the main consequences of the integration by parts formula. If one considers the *Dirac* function $\delta_x(y)$, then $\delta_x(y) = H'(y-x)$ where H is the *Heaviside* function and the above integration by parts formula reads $E(\delta_x(X)) = E(H(X-x)Q)$, where $E(\delta_x(X))$ can be interpreted as the density of the random variable X. We thus obtain an integral representation of the density of the law of X. This is the starting point of the approach to the density of the law of a diffusion process: the above integral representation allows us to prove that under appropriate hypothesis the density of X is smooth and also to derive upper and lower bounds for it. Concerning simulation by Monte Carlo methods, suppose that you want to compute $E(\delta_x(y)) \sim \frac{1}{M}\sum_{i=1}^{M}\delta_x(X^i)$ where $X^1, ..., X^M$ is a sample of X. As X has a law which is absolutely continuous with respect to the Lebesgue measure, this will fail because no X^i hits exactly x. But if you are able to simulate the weight Q as well (and this is the case in many applications because of the explicit form mentioned above) then you may try to compute $E(\delta_x(X)) = E(H(X-x)Q) \sim \frac{1}{M}\sum_{i=1}^{M}E(H(X^i-x)Q^i)$. This basic remark formula leads to efficient methods to compute by a Monte Carlo method some irregular quantities as derivatives of option prices with respect to some parameters (the *Greeks*) or conditional expectations, which appear in the pricing of American options by the dynamic programming). See the papers by Fournié et al [70] and [69] and the papers by Bally et al., Benhamou, Bermin et al., Bernis et al., Cvitanic et al., Talay and Zheng and Temam in [76].

L. Caramellino, A. Zanette and V. Bally have been concerned with the computation of conditional expectations using Integration by Parts formulas and applications to the numerical computation of the price and the Greeks (sensitivities) of American or Bermudean options. The aim of this research was to extend a paper of Reigner and Lions who treated the problem in dimension one to higher dimension - which represent the real challenge in this field. Significant results have been obtained up to dimension 5 [62] and the corresponding algorithms have been implemented in the Premia software.

Moreover, there is an increasing interest in considering jump components in the financial models, especially motivated by calibration reasons. Algorithms based on the integration by parts formulas have been developed in order to compute Greeks for options with discontinuous payoff (e.g. digital options). Several papers and two theses (M. Messaoud and M. Bavouzet defended in 2006) have been published on this topic and the corresponding algorithms have been implemented in Premia. Malliavin Calculus for jump type diffusions - and more general for random variables with locally smooth law - represents a large field of research, also for applications to credit risk problems.

The Malliavin calculus is also used in models of insider trading. The "enlargement of filtration" technique plays an important role in the modeling of such problems and the Malliavin calculus can be used to obtain general results about when and how such filtration enlargement is possible. See the paper by P. Imkeller in [76]). Moreover, in the case when the additional information of the insider is generated by adding the information about the value of one extra random variable, the Malliavin calculus can be used to find explicitly the optimal portfolio of an insider for a utility optimization problem with logarithmic utility. See the paper by J.A. León, R. Navarro and D. Nualart in [76]).

A. Kohatsu Higa and A. Sulem have studied a controlled stochastic system whose state is described by a stochastic differential equation with anticipating coefficients. These SDEs can be interpreted in the sense of *forward integrals*, which are the natural generalization of the semimartingale integrals, as introduced by Russo and Valois [84]. This methodology has been applied for utility maximization with insiders.

MCTAO Project-Team

3. Research Program

3.1. Control Systems

Our effort is directed toward efficient methods for the *control* of real (physical) systems, based on a *model* of the system to be controlled. *System* refers to the physical plant or device, whereas *model* refers to a mathematical representation of it.

We mostly investigate nonlinear systems whose nonlinearities admit a strong structure derived from physics; the equations governing their behavior are then well known, and the modeling part consists in choosing what phenomena are to be kept in the model used for control design, the other phenomena being treated as perturbations; a more complete model may be used for simulations, for instance. We focus on systems that admit a reliable finite-dimensional model, in continuous time; this means that models are controlled ordinary differential equations, often nonlinear.

Choosing accurate models yet simple enough to allow control design is in itself a key issue; however, modeling or identification as a theory is not per se in the scope of our project.

The extreme generality and versatility of linear control do not contradict the often heard sentence “most real life systems are nonlinear”. Indeed, for many control problems, a linear model is sufficient to capture the important features for control. The reason is that most control objectives are local, first order variations around an operating point or a trajectory are governed by a linear control model, and except in degenerate situations (non-controllability of this linear model), the local behavior of a nonlinear dynamic phenomenon is dictated by the behavior of first order variations. Linear control is the hard core of control theory and practice; it has been pushed to a high degree of achievement –see for instance some classics: [64], [55]– that lead to big successes in industrial applications (PID, Kalman filtering, frequency domain design, H^∞ robust control, etc...), it is taught to future engineers, and it is still a topic of ongoing research.

Linear control by itself however reaches its limits in some important situations:

1. **Non local control objectives.** Steering the system from a region to a reasonably remote other one, as in path planning and optimal control, is outside the scope of information given by a local linear approximation. It is why these are by essence nonlinear.

   Stabilisation with a basin of attraction larger than the region where the linear approximation is dominant also needs more information than one linear approximation.
2. **Local control at degenerate equilibria.** Linear control yields local stabilization of an equilibrium point based on the tangent linear approximation if the latter is controllable. It is *not* the case at interesting operating points of some physical systems; linear control is irrelevant and specific nonlinear techniques have to be designed. This is an extreme case of the second part of the above item: the region where the linear approximation is dominant vanishes.
3. **Small controls.** In some situations, actuators only allow a very small magnitude of the effect of control compared to the effect of other phenomena. Then the behavior of the system without control plays a major role and we are again outside the scope of linear control methods.

3.2. Structure of nonlinear control systems

In most problems, choosing the proper coordinates, or the right quantities that describe a phenomenon, sheds light on a path to the solution. In control systems, it is often crucial to analyze the structure of the model, deduced from physical principles, of the plant to be controlled; this may lead to putting it via some transformations in a simpler form, or a form that is most suitable for control design. For instance, equivalence to a linear system may allow to use linear control; also, the so-called “flatness” property drastically simplifies path planning [59], [70].

A better understanding of the “set of nonlinear models”, partly classifying them, has another motivation than facilitating control design for a given system and its model: it may also be a necessary step towards a theory of “nonlinear identification” and modeling. Linear identification is a mature area of control science; its success is mostly due to a very fine knowledge of the structure of the class of linear models: similarly, any progress in the understanding of the structure of the class of nonlinear models would be a contribution to a possible theory of nonlinear identification.

These topics are central in control theory, but raise very difficult mathematical questions: static feedback classification is a geometric problem which is feasible in principle, although describing invariants explicitly is technically very difficult; and conditions for dynamic feedback equivalence and linearization raise unsolved mathematical problems, that make one wonder about decidability [0].

3.3. Optimal control and feedback control, stabilization

3.3.1. *Optimal control.*

Mathematically speaking, optimal control is the modern branch of the calculus of variations, rather well established and mature [39], [68], [46], [76]. Relying on Hamiltonian dynamics is now prevalent, instead of the standard Lagrangian formalism of the calculus of variations. Also, coming from control engineering, constraints on the control (for instance the control is a force or a torque, which are naturally bounded) or the state (for example in the shuttle atmospheric re-entry problem there is a constraint on the thermal flux) are imposed; the ones on the state are usual but these on the state yield more complicated necessary optimality conditions and an increased intrinsic complexity of the optimal solutions. Also, in the modern treatment, ad-hoc numerical schemes have to be derived for effective computations of the optimal solutions.

What makes optimal control an applied field is the necessity of computing these optimal trajectories, or rather the controls that produce these trajectories (or, of course, close-by trajectories). Computing a given optimal trajectory and its control as a function of time is a demanding task, with non trivial numerical difficulties: roughly speaking, the Pontryagin Maximum Principle gives candidate optimal trajectories as solutions of a two point boundary value problem (for an ODE) which can be analyzed using mathematical tools from geometric control theory or solved numerically using shooting methods. Obtaining the *optimal synthesis* –the optimal control as a function of the state– is of course a more intricate problem [46], [51].

These questions are not only academic for minimizing a cost is *very* relevant in many control engineering problems. However, modern engineering textbooks in nonlinear control systems like the “best-seller” [61] hardly mention optimal control, and rather put the emphasis on designing a feedback control, as regular and explicit as possible, satisfying some qualitative (and extremely important!) objectives: disturbance attenuation, decoupling, output regulation or stabilization. Optimal control is sometimes viewed as disconnected from automatic control... we shall come back to this unfortunate point.

3.3.2. *Feedback, control Lyapunov functions, stabilization.*

A control Lyapunov function **(CLF)** is a function that can be made a Lyapunov function (roughly speaking, a function that decreases along all trajectories, some call this an “artificial potential”) for the closed-loop system corresponding to *some* feedback law. This can be translated into a partial differential relation sometimes called “Artstein’s (in)equation” [42]. There is a definite parallel between a CLF for stabilization, solution of this differential inequation on the one hand, and the value function of an optimal control problem for the system, solution of a HJB equation on the other hand. Now, optimal control is a quantitative objective while stabilization is a qualitative objective; it is not surprising that Artstein (in)equation is very under-determined and has many more solutions than HJB equation, and that it may (although not always) even have smooth ones.

[0] Consider the simple system with state $(x, y, z) \in I\!R^3$ and two controls that reads $\dot{z} = (\dot{y} - z\dot{x})^2\dot{x}$ after elimination of the controls; it is not known whether it is equivalent to a linear system, or flat; this is because the property amounts to existence of a formula giving the general solution as a function of two arbitrary functions of time and their derivatives up to a certain order, but no bound on this order is known a priori, even for this very particular example.

We have, in the team, a longstanding research record on the topic of construction of CLFs and stabilizing feedback controls.

3.4. Optimal Transport

We believe that matching optimal transport with geometric control theory is one originality of our team. We expect interactions in both ways.

The study of optimal mass transport problems in the Euclidean or Riemannian setting has a long history which goes from the pioneer works of Monge [72] and Kantorovitch [65] to the recent revival initiated by fundamental contributions due to Brenier [52] and McCann [71].

The same transportation problems in the presence of differential constraints on the set of paths —like being an admissible trajectory for a control system— is quite new. The first contributors were Ambrosio and Rigot [40] who proved the existence and uniqueness of an optimal transport map for the Monge problem associated with the squared canonical sub-Riemannian distance on the Heisenberg groups. This result was extended later by Agrachev and Lee [37], then by Figalli and Rifford [56] who showed that the Ambrosio-Rigot theorem holds indeed true on many sub-Riemannian manifolds satisfying reasonable assumptions. The problem of existence and uniqueness of an optimal transport map for the squared sub-Riemannian distance on a general complete sub-Riemannian manifold remains open; it is strictly related to the regularity of the sub-Riemannian distance in the product space, and remains a formidable challenge. Generalized notions of Ricci curvatures (bounded from below) in metric spaces have been developed recently by Lott and Villani [69] and Sturm [80]. A pioneer work by Juillet [62] captured the right notion of curvature for subriemannian metric in the Heisenberg group; Agrachev and Lee [38] have elaborated on this work to define new notions of curvatures in three dimensional sub-Riemannian structures. The optimal transport approach happened to be very fruitful in this context. Many things remain to be done in a more general context.

3.5. Small controls and conservative systems, averaging

Using averaging techniques to study small perturbations of integrable Hamiltonian systems dates back to H. Poincaré or earlier; it gives an approximation of the (slow) evolution of quantities that are preserved in the non-perturbed system. It is very subtle in the case of multiple periods but more elementary in the single period case, here it boils down to taking the average of the perturbation along each periodic orbit; see for instance [41], [79].

When the “perturbation” is a control, these techniques may be used after deciding how the control will depend on time and state and other quantities, for instance it may be used after applying the Pontryagin Maximum Principle as in [44], [45], [53], [60]. Without deciding the control a priori, an “average control system” may be defined as in [43].

The focus is then on studying into details this simpler “averaged” problem, that can often be described by a Riemannian metric for quadratic costs or by a Finsler metric for costs like minimum time.

This line of research stemmed out of applications to space engineering, see section 4.1 .

MEMPHIS Project-Team

3. Research Program

3.1. Hierarchical Cartesian schemes

We intend to conceive schemes that will simplify the numerical approximation of problems involving complex unsteady objects together with multi-scale physical phenomena. Rather than using extremely optimized but non-scalable algorithms, we adopt robust alternatives that bypass the difficulties linked to grid generation. Even if the mesh problem can be tackled today thanks to powerful mesh generators, it still represents a severe difficulty, in particular when highly complex unsteady geometries need to be dealt with. Industrial experience and common practice shows that mesh generation accounts for about 20% of overall analysis time, whereas creation of a simulation-specific geometry requires about 60%, and only 20% of overall time is actually devoted to analysis. The methods that we develop bypass the generation of tedious geometrical models by automatic implicit geometry representation and hierarchical Cartesian schemes.

The approach that we plan to develop combines accurate enforcement of unfitted boundary conditions with adaptive octree and overset grids. The core idea is to use an octree/overset mesh for the approximation of the solution fields, while the geometry is captured by level set functions [55], [47] and boundary conditions are imposed using appropriate interpolation methods [33], [57], [52]. This eliminates the need for boundary conforming meshes that require time-consuming and error-prone mesh generation procedures, and opens the door for simulation of very complex geometries. In particular, it will be possible to easily import the industrial geometry and to build the associated level set function used for simulation.

Hierarchical octree grids offer several considerable advantages over classical adaptive mesh refinement for body-fitted meshes, in terms of data management, memory footprint and parallel HPC performance. Typically, when refining unstructured grids, like for example tetrahedral grids, it is necessary to store the whole data tree corresponding to successive subdivisions of the elements and eventually recompute the full connectivity graph. In the linear octree case that we develop, only the tree leaves are stored in a linear array, with a considerable memory advantage. The mapping between the tree leaves and the linear array as well as the connectivity graph is efficiently computed thanks to an appropriate space-filling curve. Concerning parallelization, linear octrees guarantee a natural load balancing thanks to the linear data structure, whereas classical non-structured meshes require sophisticated (and moreover time consuming) tools to achieve proper load distribution (SCOTCH, METIS etc.). Of course, using unfitted hierarchical meshes requires further development and analysis of methods to handle the refinement at level jumps in a consistent and conservative way, accuracy analysis for new finite-volume or finite-difference schemes, efficient reconstructions at the boundaries to recover appropriate accuracy and robustness. These subjects, that are presently virtually absent at Inria, are among the main scientific challenges of our team.

3.2. Reduced-order models

Massive parallelization and rethinking of numerical schemes will allow the solution of new problem in physics and the prediction of new phenomena thanks to simulation. However, in industrial applications fast on line responses are needed for design and control. For instance, in the design process of an aircraft, the flight conditions and manoeuvres, which provide the largest aircraft loads, are not known a priori. Therefore the aerodynamic and inertial forces are calculated at a large number of conditions to give an estimate of the maximum loads, and hence stresses, that the structure of the detailed aircraft design will experience in service. A simplistic estimate of the number of analyses required would multiply the numbers of conditions to give 10^7. Even with simplistic models of the aircraft behavior this is an unfeasible number of separate simulations. However, engineering experience is used to identify the most likely critical loads conditions, meaning that approximately 10^5 simulations are required for conventional aircraft configurations. Furthermore these analyses have to be repeated every time that there is an update in the aircraft structure...

Compared to existing approaches for ROMs [44], our interest will be focused on two axis. On the one hand, we start from the consideration that small, highly non-linear scales are typically concentrated in limited spatial regions of the full simulation domain. So for example, in the flow past a wing, the highly non-linear phenomena take place close to the walls at the scale of a millimeter for computational domains that are of the order of hundreds of meters. In this context our approach is characterized by a multi-scale model where the large scales are described by far field models based on ROMs and the small scales are simulated by high-fidelity models. The whole point for this approach is to optimally decouple the far field from the near field.

A second characterizing feature of our ROM approach is non-linear interpolation. We start from the consideration that dynamical models derived from the projection of the PDE model in the reduced space are neither stable to numerical integration nor robust to parameter variation when hard non-linear multi-scale phenomena are considered.

However, thanks to Proper Orthogonal Decomposition (POD) [48], [56], [36] we can accurately approximate large solution databases using a small base. Recent techniques to investigate the temporal evolution of the POD modes (Koopman modes [50], [34], Dynamic Mode Decomposition [54]) allow a dynamic discrimination of the role played by each of them. This in turn can be exploited to interpolate between the modes in parameter space, thanks to ideas relying on optimal transportation [58], [40] that we have started developing in the FP7 project FFAST and H2020 AEROGUST. In the following we precise these ideas on a specific example.

MEPHYSTO Project-Team

3. Research Program

3.1. From statistical physics to continuum mechanics

Whereas numerical methods in nonlinear elasticity are well-developed and reliable, constitutive laws used for rubber in practice are phenomenological and generally not very precise. On the contrary, at the scale of the polymer-chain network, the physics of rubber is very precisely described by statistical physics. The main challenge in this field is to understand how to derive macroscopic constitutive laws for rubber-like materials from statistical physics.

At the continuum level, rubber is modelled by an energy E defined as the integral over a domain D of $\mathbb{R}^d$ of some energy density W depending only locally on the gradient of the deformation u: $E(u) = \int_D W(\nabla u(x))dx$. At the microscopic level (say 100nm), rubber is a network of cross-linked and entangled polymer chains (each chain is made of a sequence of monomers). At this scale the physics of polymer chains is well-understood in terms of statistical mechanics: monomers thermally fluctuate according to the Boltzmann distribution [63]. The associated Hamiltonian of a network is typically given by a contribution of the polymer chains (using self-avoiding random bridges) and a contribution due to steric effects (rubber is packed and monomers are surrounded by an excluded volume). The main challenge is to understand how this statistical physics picture yields rubber elasticity. Treloar assumed in [77] that for a piece of rubber undergoing some macroscopic deformation, the cross-links do not fluctuate and follow the macroscopic deformation, whereas between two cross-links, the chains fluctuate. This is the so-called affine assumption. Treloar's model is in rather good agreement with mechanical experiments in small deformation. In large deformation however, it overestimates the stress. A natural possibility to relax Treloar's model consists in relaxing the affine assumption while keeping the network description, which allows one to distinguish between different rubbers. This can be done by assuming that the deformation of the cross-links minimizes the free energy of the polymer chains, the deformation being fixed at the boundary of the macroscopic domain D. This gives rise to a “variational model". The analysis of the asymptotic behavior of this model as the typical length of a polymer chain vanishes has the same flavor as the homogenization theory of integral functionals in nonlinear elasticity (see [55], [73] in the periodic setting, and [56] in the random setting).

Our aim is to relate qualitatively and quantitatively the (precise but unpractical) statistical physics picture to explicit macroscopic constitutive laws that can be used for practical purposes.

In collaboration with R. Alicandro (Univ. Cassino, Italy) and M. Cicalese (Univ. Munich, Germany), A. Gloria analyzed in [1] the (asymptotic) Γ-convergence of the variational model for rubber, in the case when the polymer chain network is represented by some ergodic random graph. The easiest such graph is the Delaunay tessellation of a point set generated as follows: random hard spheres of some given radius ρ are picked randomly until the domain is jammed (the so-called random parking measure of intensity ρ). With M. Penrose (Univ. Bath, UK), A. Gloria studied this random graph in this framework [5]. With P. Le Tallec (Mechanics department, Ecole polytechnique, France), M. Vidrascu (project-team REO, Inria Paris-Rocquencourt), and A. Gloria introduced and tested in [65] a numerical algorithm to approximate the homogenized energy density, and observed that this model compares well to rubber elasticity qualitatively.

These preliminary results show that the variational model has the potential to explain qualitatively and quantitatively how rubber elasticity emerges from polymer physics. In order to go further and obtain more quantitative results and rigorously justify the model, we have to address several questions of analysis, modelling, scientific computing, inverse problems, and physics.

3.2. Quantitative stochastic homogenization

Whereas the approximation of homogenized coefficients is an easy task in periodic homogenization, this is a highly nontrivial task for stochastic coefficients. This is in order to analyze numerical approximation methods of the homogenized coefficients that F. Otto (MPI for mathematics in the sciences, Leipzig, Germany) and A. Gloria obtained the first quantitative results in stochastic homogenization [3]. The development of a complete stochastic homogenization theory seems to be ripe for the analysis and constitutes the second major objective of this section.

In order to develop a quantitative theory of stochastic homogenization, one needs to quantitatively understand the corrector equation (3). Provided A is stationary and ergodic, it is known that there exists a unique random field ϕ_ξ which is a distributional solution of (3) almost surely, such that $\nabla\phi_\xi$ is a stationary random field with bounded second moment $\left\langle|\nabla\phi_\xi|^2\right\rangle<\infty$, and with $\phi(0)=0$. Soft arguments do not allow to prove that ϕ_ξ may be chosen stationary (this is wrong in dimension $d=1$). In [3], [4] F. Otto and A. Gloria proved that, in the case of discrete elliptic equations with iid conductances, there exists a unique stationary corrector ϕ_ξ with vanishing expectation in dimension $d>2$. Although it cannot be bounded, it has bounded finite moments of any order:

$$\langle|\phi_\xi|^q\rangle<\infty \text{ for all } q\geq 1. \tag{59}$$

They also proved that the variance of spatial averages of the energy density $(\xi+\nabla\phi_\xi)\cdot A(\xi+\nabla\phi_\xi)$ on balls of radius R decays at the rate R^{-d} of the central limit theorem. These are the *first optimal quantitative results* in stochastic homogenization.

The proof of these results, which is inspired by [74], is based on the insight that coefficients such as the Poisson random inclusions are special in the sense that the associated probability measure satisfies a spectral gap estimate. Combined with elliptic regularity theory, this spectral gap estimate quantifies ergodicity in stochastic homogenization. This systematic use of tools from statistical physics has opened the way to the quantitative study of stochastic homogenization problems, which we plan to fully develop.

3.3. Nonlinear Schrödinger equations

As well known, the (non)linear Schrödinger equation

$$\partial_t\varphi(t,x)=-\Delta\varphi(t,x)+\lambda V(x)\varphi(t,x)+g|\varphi|^2\varphi(t,x),\quad \varphi(0,x)=\varphi_0(x) \tag{60}$$

with coupling constants $g\in\mathbb{R}, \lambda\in\mathbb{R}_+$ and real potential V (possibly depending also on time) models many phenomena of physics.

When in the equation (5) above one sets $\lambda=0, g\neq 0$, one obtains the nonlinear (focusing of defocusing) Schrödinger equation. It is used to model light propagation in optical fibers. In fact, it then takes the following form:

$$i\partial_z\varphi(t,z)=-\beta(z)\partial_t^2\varphi(t,z)+\gamma(z)|\varphi(t,z)|^2\varphi(z,t), \tag{61}$$

where β and γ are functions that characterize the physical properties of the fiber, t is time and z the position along the fiber. Several issues are of importance here. Two that will be investigated within the MEPHYSTO project are: the influence of a periodic modulation of the fiber parameters β and γ and the generation of so-called “rogue waves” (which are solutions of unusually high amplitude) in such systems.

If $g = 0, \lambda \neq 0$, V is a random potential, and φ_0 is deterministic, this is the standard random Schrödinger equation describing for example the motion of an electron in a random medium. The main issue in this setting is the determination of the regime of Anderson localization, a property characterized by the boundedness in time of the second moment $\int x^2 |\varphi(t,x)|^2 dx$ of the solution. If this second moment remains bounded in time, the solution is said to be localized. Whereas it is known that the solution is localized in one dimension for all (suitable) initial data, both localized and delocalized solutions exist in dimension 3 and it remains a major open problem today to prove this, cf. [61].

If now $g \neq 0, \lambda \neq 0$ and V is still random, but $|g| \ll \lambda$, a natural question is whether, and in which regime, one-dimensional Anderson localization perdures. Indeed, Anderson localization can be affected by the presence of the nonlinearity, which corresponds to an interaction between the electrons or atoms. Much numerical and some analytical work has been done on this issue (see for example [64] for a recent work at PhLAM, Laser physics department, Univ. Lille 1), but many questions remain, notably on the dependence of the result on the initial conditions, which, in a nonlinear system, may be very complex. The cold atoms team of PhLAM (Garreau-Szriftgiser) is currently setting up an experiment to analyze the effect of the interactions in a Bose-Einstein condensate on a closely related localization phenomenon called “dynamical localization”, in the kicked rotor, see below.

3.4. Processes in random environment

In the course of developing a quantitative theory of stochastic homogenization of discrete elliptic equations, we have introduced new tools to quantify ergodicity in partial differential equations. These tools are however not limited to PDEs, and could also have an impact in other fields where an evolution takes place in a (possibly dynamic) random environment and an averaging process occurs. The goal is then to understand the asymptotics of the motion of the particle/process.

For a random walker in a random environment, the Kipnis-Varadhan theorem ensures that the expected squared-position of the random walker after time t is of order t (the prefactor depends on the homogenized coefficients). If instead of a random walk among random conductances we consider a particle with some initial velocity evolving in a random *potential* field according to the Newton law, the averaged squared-position at time t is expected to follow the scaling law t^2, see [44]. This is called stochastic acceleration.

Similar questions arise when the medium is reactive (that is, when the potential is modified by the particle itself). The approach to equilibrium in such systems was observed numerically and explained theoretically, but not completely proven, in [58].

Another related and more general direction of research is the validity of *universality principle* of statistical physics, which states that the qualitative behaviour of physical systems depend on the microscopic details of the system only through some large-scale variables (the thermodynamic variables). Therefore, it is a natural problem in the field of interacting particle systems to obtain the macroscopic laws of the relevant thermodynamical quantities, using an underlying microscopic dynamics, namely particles that move according to some prescribed stochastic law. Probabilistically speaking, these systems are continuous time Markov processes.

MISTIS Project-Team

3. Research Program

3.1. Mixture models

Participants: Alexis Arnaud, Jean-Baptiste Durand, Florence Forbes, Aina Frau Pascual, Alessandro Chiancone, Stephane Girard, Julyan Arbel, Gildas Mazo, Jean-Michel Becu.

Key-words: mixture of distributions, EM algorithm, missing data, conditional independence, statistical pattern recognition, clustering, unsupervised and partially supervised learning.

In a first approach, we consider statistical parametric models, θ being the parameter, possibly multi-dimensional, usually unknown and to be estimated. We consider cases where the data naturally divides into observed data $y = \{y_1, ..., y_n\}$ and unobserved or missing data $z = \{z_1, ..., z_n\}$. The missing data z_i represents for instance the memberships of one of a set of K alternative categories. The distribution of an observed y_i can be written as a finite mixture of distributions,

$$f(y_i;\theta) = \sum_{k=1}^{K} P(z_i = k;\theta) f(y_i \mid z_i;\theta) \; . \tag{62}$$

These models are interesting in that they may point out hidden variables responsible for most of the observed variability and so that the observed variables are *conditionally* independent. Their estimation is often difficult due to the missing data. The Expectation-Maximization (EM) algorithm is a general and now standard approach to maximization of the likelihood in missing data problems. It provides parameter estimation but also values for missing data.

Mixture models correspond to independent z_i's. They have been increasingly used in statistical pattern recognition. They enable a formal (model-based) approach to (unsupervised) clustering.

3.2. Markov models

Participants: Brice Olivier, Thibaud Rahier, Jean-Baptiste Durand, Florence Forbes, Karina Ashurbekova.

Key-words: graphical models, Markov properties, hidden Markov models, clustering, missing data, mixture of distributions, EM algorithm, image analysis, Bayesian inference.

Graphical modelling provides a diagrammatic representation of the dependency structure of a joint probability distribution, in the form of a network or graph depicting the local relations among variables. The graph can have directed or undirected links or edges between the nodes, which represent the individual variables. Associated with the graph are various Markov properties that specify how the graph encodes conditional independence assumptions.

It is the conditional independence assumptions that give graphical models their fundamental modular structure, enabling computation of globally interesting quantities from local specifications. In this way graphical models form an essential basis for our methodologies based on structures.

The graphs can be either directed, e.g. Bayesian Networks, or undirected, e.g. Markov Random Fields. The specificity of Markovian models is that the dependencies between the nodes are limited to the nearest neighbor nodes. The neighborhood definition can vary and be adapted to the problem of interest. When parts of the variables (nodes) are not observed or missing, we refer to these models as Hidden Markov Models (HMM). Hidden Markov chains or hidden Markov fields correspond to cases where the z_i's in (1) are distributed according to a Markov chain or a Markov field. They are a natural extension of mixture models. They are widely used in signal processing (speech recognition, genome sequence analysis) and in image processing (remote sensing, MRI, etc.). Such models are very flexible in practice and can naturally account for the phenomena to be studied.

Hidden Markov models are very useful in modelling spatial dependencies but these dependencies and the possible existence of hidden variables are also responsible for a typically large amount of computation. It follows that the statistical analysis may not be straightforward. Typical issues are related to the neighborhood structure to be chosen when not dictated by the context and the possible high dimensionality of the observations. This also requires a good understanding of the role of each parameter and methods to tune them depending on the goal in mind. Regarding estimation algorithms, they correspond to an energy minimization problem which is NP-hard and usually performed through approximation. We focus on a certain type of methods based on variational approximations and propose effective algorithms which show good performance in practice and for which we also study theoretical properties. We also propose some tools for model selection. Eventually we investigate ways to extend the standard Hidden Markov Field model to increase its modelling power.

3.3. Functional Inference, semi- and non-parametric methods

Participants: Clement Albert, Alessandro Chiancone, Stephane Girard, Seydou Nourou Sylla, Pablo Mesejo Santiago, Florence Forbes, Emeline Perthame, Jean-Michel Becu.

Key-words: dimension reduction, extreme value analysis, functional estimation.

We also consider methods which do not assume a parametric model. The approaches are non-parametric in the sense that they do not require the assumption of a prior model on the unknown quantities. This property is important since, for image applications for instance, it is very difficult to introduce sufficiently general parametric models because of the wide variety of image contents. Projection methods are then a way to decompose the unknown quantity on a set of functions (*e.g.* wavelets). Kernel methods which rely on smoothing the data using a set of kernels (usually probability distributions) are other examples. Relationships exist between these methods and learning techniques using Support Vector Machine (SVM) as this appears in the context of *level-sets estimation* (see section 3.3.2). Such non-parametric methods have become the cornerstone when dealing with functional data [77]. This is the case, for instance, when observations are curves. They enable us to model the data without a discretization step. More generally, these techniques are of great use for *dimension reduction* purposes (section 3.3.3). They enable reduction of the dimension of the functional or multivariate data without assumptions on the observations distribution. Semi-parametric methods refer to methods that include both parametric and non-parametric aspects. Examples include the Sliced Inverse Regression (SIR) method [80] which combines non-parametric regression techniques with parametric dimension reduction aspects. This is also the case in *extreme value analysis* [76], which is based on the modelling of distribution tails (see section 3.3.1). It differs from traditional statistics which focuses on the central part of distributions, *i.e.* on the most probable events. Extreme value theory shows that distribution tails can be modelled by both a functional part and a real parameter, the extreme value index.

3.3.1. Modelling extremal events

Extreme value theory is a branch of statistics dealing with the extreme deviations from the bulk of probability distributions. More specifically, it focuses on the limiting distributions for the minimum or the maximum of a large collection of random observations from the same arbitrary distribution. Let $X_{1,n} \leq ... \leq X_{n,n}$ denote n ordered observations from a random variable X representing some quantity of interest. A p_n-quantile of X is the value x_{p_n} such that the probability that X is greater than x_{p_n} is p_n, *i.e.*$P(X > x_{p_n}) = p_n$. When $p_n < 1/n$, such a quantile is said to be extreme since it is usually greater than the maximum observation $X_{n,n}$ (see Figure 1).

To estimate such quantiles therefore requires dedicated methods to extrapolate information beyond the observed values of X. Those methods are based on Extreme value theory. This kind of issue appeared in hydrology. One objective was to assess risk for highly unusual events, such as 100-year floods, starting from flows measured over 50 years. To this end, semi-parametric models of the tail are considered:

$$P(X > x) = x^{-1/\theta}\ell(x),\ x > x_0 > 0, \tag{63}$$

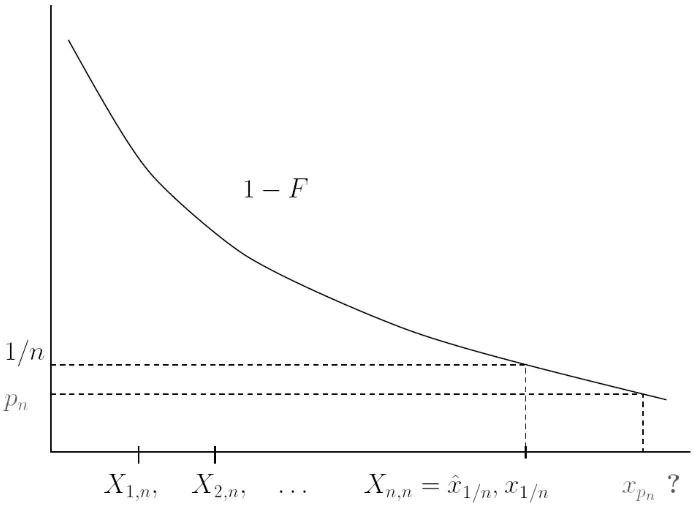


Figure 1. The curve represents the survival function $x \to P(X > x)$. The $1/n$-quantile is estimated by the maximum observation so that $\widehat{x}_{1/n} = X_{n,n}$. As illustrated in the figure, to estimate p_n-quantiles with $p_n < 1/n$, it is necessary to extrapolate beyond the maximum observation.

where both the extreme-value index $\theta > 0$ and the function $\ell(x)$ are unknown. The function ℓ is a slowly varying function *i.e.* such that

$$\frac{\ell(tx)}{\ell(x)} \to 1 \text{ as } x \to \infty \tag{64}$$

for all $t > 0$. The function $\ell(x)$ acts as a nuisance parameter which yields a bias in the classical extreme-value estimators developed so far. Such models are often referred to as heavy-tail models since the probability of extreme events decreases at a polynomial rate to zero. It may be necessary to refine the model (2 ,3) by specifying a precise rate of convergence in (3). To this end, a second order condition is introduced involving an additional parameter $\rho \leq 0$. The larger ρ is, the slower the convergence in (3) and the more difficult the estimation of extreme quantiles.

More generally, the problems that we address are part of the risk management theory. For instance, in reliability, the distributions of interest are included in a semi-parametric family whose tails are decreasing exponentially fast. These so-called Weibull-tail distributions [9] are defined by their survival distribution function:

$$P(X > x) = \exp\{-x^{\theta}\ell(x)\},\ x > x_0 > 0. \tag{65}$$

Gaussian, gamma, exponential and Weibull distributions, among others, are included in this family. An important part of our work consists in establishing links between models (2) and (4) in order to propose new estimation methods. We also consider the case where the observations were recorded with a covariate information. In this case, the extreme-value index and the p_n-quantile are functions of the covariate. We propose estimators of these functions by using moving window approaches, nearest neighbor methods, or kernel estimators.

3.3.2. Level sets estimation

Level sets estimation is a recurrent problem in statistics which is linked to outlier detection. In biology, one is interested in estimating reference curves, that is to say curves which bound 90% (for example) of the population. Points outside this bound are considered as outliers compared to the reference population. Level sets estimation can be looked at as a conditional quantile estimation problem which benefits from a non-parametric statistical framework. In particular, boundary estimation, arising in image segmentation as well as in supervised learning, is interpreted as an extreme level set estimation problem. Level sets estimation can also be formulated as a linear programming problem. In this context, estimates are sparse since they involve only a small fraction of the dataset, called the set of support vectors.

3.3.3. Dimension reduction

Our work on high dimensional data requires that we face the curse of dimensionality phenomenon. Indeed, the modelling of high dimensional data requires complex models and thus the estimation of high number of parameters compared to the sample size. In this framework, dimension reduction methods aim at replacing the original variables by a small number of linear combinations with as small as a possible loss of information. Principal Component Analysis (PCA) is the most widely used method to reduce dimension in data. However, standard linear PCA can be quite inefficient on image data where even simple image distorsions can lead to highly non-linear data. Two directions are investigated. First, non-linear PCAs can be proposed, leading to semi-parametric dimension reduction methods [78]. Another field of investigation is to take into account the application goal in the dimension reduction step. One of our approaches is therefore to develop new Gaussian models of high dimensional data for parametric inference [74]. Such models can then be used in a Mixtures or Markov framework for classification purposes. Another approach consists in combining dimension reduction, regularization techniques, and regression techniques to improve the Sliced Inverse Regression method [80].

MODAL Project-Team

3. Research Program

3.1. Generative model design

The first objective of MODAL consists in designing, analyzing, estimating and evaluating new generative parametric models for multivariate and/or heterogeneous data. It corresponds typically to continuous and categorical data but it includes also other widespread ones like ordinal, functional, ranks,...Designed models have to take into account potential correlations between variables while being (1) justifiable and realistic, (2) meaningful and parsimoniously parameterized, (3) of low computational complexity. The main purpose is to identify a few theoretical and general principles for model generation, loosely dependent on the variable nature. In this context, we propose two concurrent approaches which could be general enough for dealing with correlation between many types of homogeneous or heterogeneous variables:

- Designs general models by combining two extreme models (full dependent and full independent) which are well-defined for most of variables;
- Uses kernels as a general way for dealing with multivariate and heterogeneous variables.

3.2. Data visualization

The second objective of MODAL is to propose meaningful and quite accurate low dimensional visualizations of data typically in two-dimensional (2D) spaces, less frequently in one-dimensional (1D) or three-dimensional (3D) spaces, by using the generative models designed in the first objective. We propose also to visualize simultaneously the data and the model. All visualizations will depend on the aim at hand (typically clustering, classification or density estimation). The main originality of this objective lies in the use of models for visualization, a strategy from which we expect to have a better control on the subjectivity necessarily induced by any graphical display. In addition, the proposed approach has to be general enough to be independent on the variable nature. Note that the visualization objective is consistent with the dissemination of our methodologies through specific softwares. Indeed, displaying data is an important step in the data analysis process.

MOKAPLAN Project-Team

3. Research Program

3.1. Modeling and Analysis

The first layer of methodological tools developed by our team is a set of theoretical continuous models that aim at formalizing the problems studied in the applications. These theoretical findings will also pave the way to efficient numerical solvers that are detailed in Section 3.2 .

3.1.1. Static Optimal Transport and Generalizations

3.1.1.1. Convexity constraint and Principal Agent problem in Economics.

(*Participants:* G. Carlier, J-D. Benamou, V. Duval, Xavier Dupuis (LUISS Guido Carli University, Roma)) The principal agent problem plays a distinguished role in the literature on asymmetric information and contract theory (with important contributions from several Nobel prizes such as Mirrlees, Myerson or Spence) and it has many important applications in optimal taxation, insurance, nonlinear pricing. The typical problem consists in finding a cost minimizing strategy for a monopolist facing a population of agents who have an unobservable characteristic, the principal therefore has to take into account the so-called incentive compatibilty constraint which is very similar to the cyclical monotonicity condition which characterizes optimal transport plans. In a special case, Rochet and Choné [169] reformulated the problem as a variational problem subject to a convexity constraint. For more general models, and using ideas from Optimal Transportation, Carlier [98] considered the more general c-convexity constraint and proved a general existence result. Using the formulation of [98] McCann, Figalli and Kim [124] gave conditions under which the principal agent problem can be written as an infinite dimensional convex variational problem. The important results of [124] are intimately connected to the regularity theory for optimal transport and showed that there is some hope to numerically solve the principal-agent problem for general utility functions.

Our expertise: We have already contributed to the numerical resolution of the Principal Agent problem in the case of the convexity constraint, see [104], [157], [154].

Goals: So far, the mathematical PA model can be numerically solved for simple utility functions. A Bregman approach inspired by [64] is currently being developed [101] for more general functions. It would be extremely useful as a complement to the theoretical analysis. A new semi-Discrete Geometric approach is also investigated where the method reduces to non-convex polynomial optimization.

3.1.1.2. Optimal transport and conditional constraints in statistics and finance.

(*Participants:* G. Carlier, J-D. Benamou, G. Peyré) A challenging branch of emerging generalizations of Optimal Transportation arising in *economics, statistics and finance* concerns Optimal Transportation with *conditional* constraints. The *martingale optimal transport* [58], [129] which appears naturally in mathematical finance aims at computing robust bounds on option prices as the value of an optimal transport problem where not only the marginals are fixed but the coupling should be the law of a martingale, since it represents the prices of the underlying asset under the risk-neutral probability at the different dates. Note that as soon as more than two dates are involved, we are facing a multimarginal problem.

Our expertise: Our team has a deep expertise on the topic of OT and its generalization, including many already existing collaboration between its members, see for instance [64], [69], [62] for some representative recent collaborative publications.

Goals: This is a non trivial extension of Optimal Transportation theory and MOKAPLAN will develop numerical methods (in the spirit of entropic regularization) to address it. A popular problem in statistics is the so-called quantile regression problem, recently Carlier, Chernozhukov and Galichon [99] used an Optimal Transportation approach to extend quantile regression to several dimensions. In this approach again, not only fixed marginals constraints are present but also constraints on conditional means. As in the martingale Optimal Transportation problem, one has to deal with an extra conditional constraint. The usual duality approach usually breaks down under such constraints and characterization of optimal couplings is a challenging task both from a theoretical and numerical viewpoint.

3.1.1.3. JKO gradient flows.

(*Participants:* G. Carlier, J-D. Benamou, M. Laborde, Q. Mérigot, V. Duval) The connection between the static and dynamic transportation problems (see Section 2.3) opens the door to many extensions, most notably by leveraging the use of gradient flows in metric spaces. The flow with respect to the transportation distance has been introduced by Jordan-Kindelherer-Otto (JKO) [137] and provides a variational formulation of many linear and non-linear diffusion equations. The prototypical example is the Fokker Planck equation. We will explore this formalism to study new variational problems over probability spaces, and also to derive innovative numerical solvers. The JKO scheme has been very successfully used to study evolution equations that have the structure of a gradient flow in the Wasserstein space. Indeed many important PDEs have this structure: the Fokker-Planck equation (as was first considered by [137]), the porous medium equations, the granular media equation, just to give a few examples. It also finds application in image processing [87]. Figure 4 shows examples of gradient flows.

Our expertise: There is an ongoing collaboration between the team members on the theoretical and numerical analysis of gradient flows.

Goals: We apply and extend our research on JKO numerical methods to treat various extensions:

- Wasserstein gradient flows with a non displacement convex energy (as in the parabolic-elliptic Keller-Segel chemotaxis model [107])
- systems of evolution equations which can be written as gradient flows of some energy on a product space (possibly mixing the Wasserstein and L^2 structures) : multi-species models or the parabolic-parabolic Keller-Segel model [74]
- perturbation of gradient flows: multi-species or kinetic models are not gradient flows, but may be viewed as a perturbation of Wasserstein gradient flows, we shall therefore investigate convergence of splitting methods for such equations or systems.

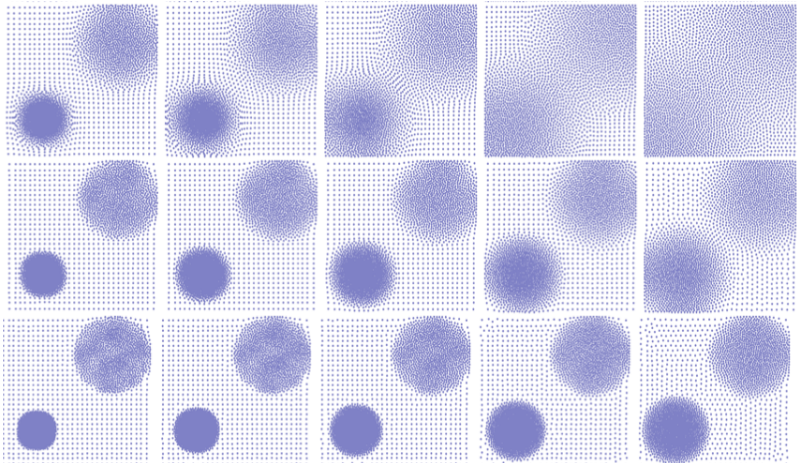


Figure 4. Example of non-linear diffusion equations solved with a JKO flow [65]. The horizontal axis shows the time evolution minimizing the functional $\int \frac{\rho^\alpha}{\alpha-1}$ on the density ρ (discretized here using point clouds, i.e. sum of Diracs' with equal mass). Each row shows a different value of $\alpha = (0.6, 2, 3)$

3.1.1.4. From networks to continuum congestion models.

(*Participants:* G. Carlier, J-D. Benamou, G. Peyré) Congested transport theory in the discrete framework of networks has received a lot of attention since the 50's starting with the seminal work of Wardrop. A few years later, Beckmann proved that equilibria are characterized as solution of a convex minimization problem. However, this minimization problem involves one flow variable per path on the network, its dimension thus quickly becomes too large in practice. An alternative, is to consider continuous in space models of congested optimal transport as was done in [103] which leads to very degenerate PDEs [79].

Our expertise: MOKAPLAN members have contributed a lot to the analysis of congested transport problems and to optimization problems with respect to a metric which can be attacked numerically by fast marching methods [69].

Goals: The case of general networks/anisotropies is still not well understood, general Γ-convergence results will be investigated as well as a detailed analysis of the corresponding PDEs and numerical methods to solve them. Benamou and Carlier already studied numerically some of these PDEs by an augmented Lagrangian method see figure 5 . Note that these class of problems share important similarities with metric learning problem in machine learning, detailed in Section 4.2 .

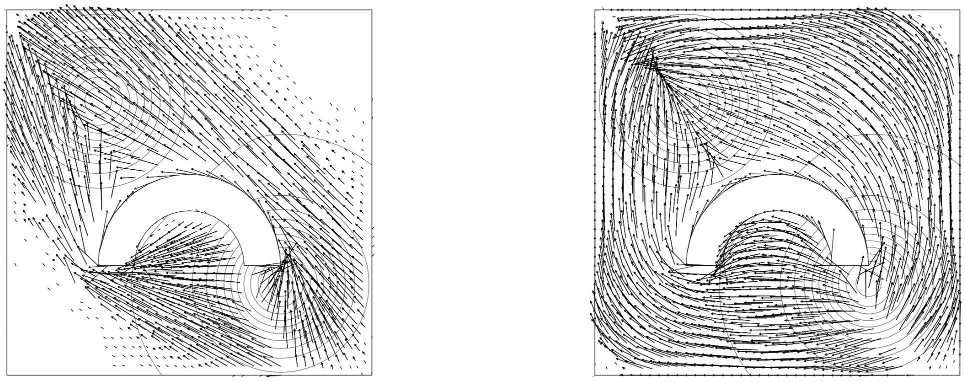


Figure 5. Monge and Wardrop flows of mass around an obstacle [62]. the source/target mass is represented by the level curves. Left : no congestion, Right : congestion.

3.1.2. Diffeomorphisms and Dynamical Transport

3.1.2.1. Growth Models for Dynamical Optimal Transport.

(*Participants:* F-X. Vialard, J-D. Benamou, G. Peyré, L. Chizat) A major issue with the standard dynamical formulation of OT is that it does not allow for variation of mass during the evolution, which is required when tackling medical imaging applications such as tumor growth modeling [90] or tracking elastic organ movements [174]. Previous attempts [148], [165] to introduce a source term in the evolution typically lead to mass teleportation (propagation of mass with infinite speed), which is not always satisfactory.

Our expertise: Our team has already established key contributions both to connect OT to fluid dynamics [60] and to define geodesic metrics on the space of shapes and diffeomorphisms [111].

Goals: Lenaic Chizat's PhD thesis aims at bridging the gap between dynamical OT formulation, and LDDDM diffeomorphisms models (see Section 2.3). This will lead to biologically-plausible evolution models that are both more tractable numerically than LDDM competitors, and benefit from strong theoretical guarantees associated to properties of OT.

3.1.2.2. Mean-field games.

(*Participants:* G. Carlier, J-D. Benamou) The Optimal Transportation Computational Fluid Dynamics (CFD) formulation is a limit case of variational Mean-Field Games (MFGs), a new branch of game theory recently developed by J-M. Lasry and P-L. Lions [141] with an extremely wide range of potential applications [132]. Non-smooth proximal optimization methods used successfully for the Optimal Transportation can be used in the case of deterministic MFGs with singular data and/or potentials [63]. They provide a robust treatment of the positivity constraint on the density of players.

Our expertise: J.-D. Benamou has pioneered with Brenier the CFD approach to Optimal Transportation. Regarding MFGs, on the numerical side, our team has already worked on the use of augmented Lagrangian methods in MFGs [62] and on the analytical side [97] has explored rigorously the optimality system for a singular CFD problem similar to the MFG system.

Goals: We will work on the extension to stochastic MFGs. It leads to non-trivial numerical difficulties already pointed out in [50].

3.1.2.3. Macroscopic Crowd motion, congestion and equilibria.

(*Participants:* G. Carlier, J-D. Benamou, Q. Mérigot, F. Santambrogio (U. Paris-Sud), Y. Achdou (Univ. Paris 7), R. Andreev (Univ. Paris 7)) Many models from PDEs and fluid mechanics have been used to give a description of *people or vehicles moving in a congested environment*. These models have to be classified according to the dimension (1D model are mostly used for cars on traffic networks, while 2-D models are most suitable for pedestrians), to the congestion effects ("soft" congestion standing for the phenomenon where high densities slow down the movement, "hard" congestion for the sudden effects when contacts occur, or a certain threshold is attained), and to the possible rationality of the agents Maury et al [152] recently developed a theory for 2D hard congestion models without rationality, first in a discrete and then in a continuous framework. This model produces a PDE that is difficult to attack with usual PDE methods, but has been successfully studied via Optimal Transportation techniques again related to the JKO gradient flow paradigm. Another possibility to model crowd motion is to use the mean field game approach of Lions and Lasry which limits of Nash equilibria when the number of players is large. This also gives macroscopic models where congestion may appear but this time a global equilibrium strategy is modelled rather than local optimisation by players like in the JKO approach. Numerical methods are starting to be available, see for instance [50], [86].

Our expertise: We have developed numerical methods to tackle both the JKO approach and the MFG approach. The Augmented Lagrangian (proximal) numerical method can actually be applied to both models [62], JKO and deterministic MFGs.

Goals: We want to extend our numerical approach to more realistic congestion model where the speed of agents depends on the density, see Figure 6 for preliminary results. Comparison with different numerical approaches will also be performed inside the ANR ISOTACE. Extension of the Augmented Lagrangian approach to Stochastic MFG will be studied.

3.1.2.4. Diffeomorphic image matching.

(*Participants:* F-X. Vialard, G. Peyré, B. Schmitzer, L. Chizat) Diffeomorphic image registration is widely used in medical image analysis. This class of problems can be seen as the computation of a generalized optimal transport, where the optimal path is a geodesic on a group of diffeomorphisms. The major difference between the two approaches being that optimal transport leads to non smooth optimal maps in general, which is however compulsory in diffeomorphic image matching. In contrast, optimal transport enjoys a convex variational formulation whereas in LDDMM the minimization problem is non convex.

Our expertise: F-X. Vialard is an expert of diffeomorphic image matching (LDDMM) [180], [85], [178]. Our team has already studied flows and geodesics over non-Riemannian shape spaces, which allows for piecewise smooth deformations [111].

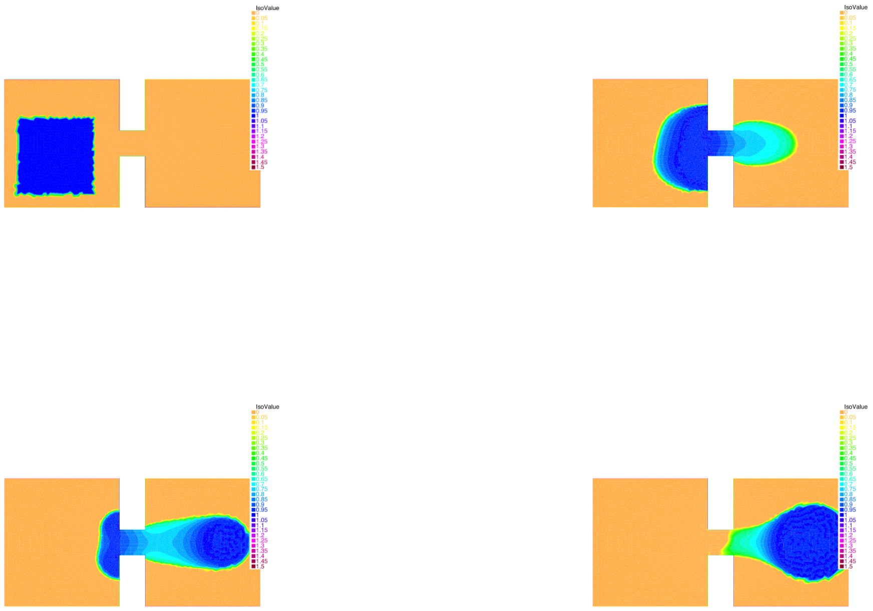


Figure 6. Example of crowd congestion with density dependent speed. The macroscopic density, at 4 different times, of people forced to exit from one room towards a meeting point in a second room.

Goals: Our aim consists in bridging the gap between standard optimal transport and diffeomorphic methods by building new diffeomorphic matching variational formulations that are convex (geometric obstructions might however appear). A related perspective is the development of new registration/transport models in a Lagrangian framework, in the spirit of [173], [174] to obtain more meaningful statistics on longitudinal studies.

Diffeomorphic matching consists in the minimization of a functional that is a sum of a deformation cost and a similarity measure. The choice of the similarity measure is as important as the deformation cost. It is often chosen as a norm on a Hilbert space such as functions, currents or varifolds. From a Bayesian perspective, these similarity measures are related to the noise model on the observed data which is of geometric nature and it is not taken into account when using Hilbert norms. Optimal transport fidelity have been used in the context of signal and image denoising [143], and it is an important question to extends these approach to registration problems. Therefore, we propose to develop similarity measures that are geometric and computationally very efficient using entropic regularization of optimal transport.

Our approach is to use a regularized optimal transport to design new similarity measures on all of those Hilbert spaces. Understanding the precise connections between the evolution of shapes and probability distributions will be investigated to cross-fertilize both fields by developing novel transportation metrics and diffeomorphic shape flows.

The corresponding numerical schemes are however computationally very costly. Leveraging our understanding of the dynamic optimal transport problem and its numerical resolution, we propose to develop new algorithms. These algorithms will use the smoothness of the Riemannian metric to improve both accuracy and speed, using for instance higher order minimization algorithm on (infinite dimensional) manifolds.

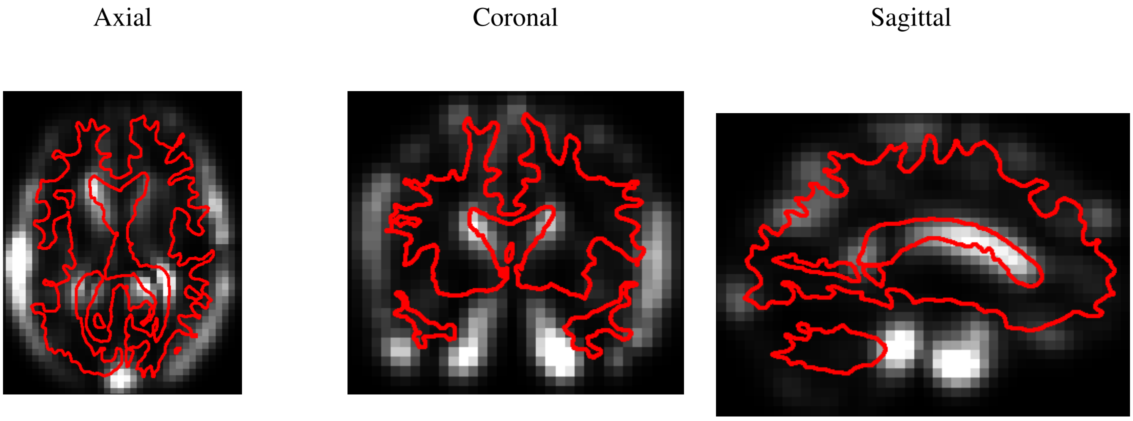
3.1.2.5. Metric learning and parallel transport for statistical applications.

(*Participants:* F-X. Vialard, G. Peyré, B. Schmitzer, L. Chizat) The LDDMM framework has been advocated to enable statistics on the space of shapes or images that benefit from the estimation of the deformation. The statistical results of it strongly depend on the choice of the Riemannian metric. A possible direction consists in learning the right invariant Riemannian metric as done in [181] where a correlation matrix (Figure 7) is learnt which represents the covariance matrix of the deformation fields for a given population of shapes. In the same direction, a question of emerging interest in medical imaging is the analysis of time sequence of shapes (called longitudinal analysis) for early diagnosis of disease, for instance [125]. A key question is the inter subject comparison of the organ evolution which is usually done by transport of the time evolution in a common coordinate system via parallel transport or other more basic methods. Once again, the statistical results (Figure 8) strongly depend on the choice of the metric or more generally on the connection that defines parallel transport.
Our expertise: Our team has already studied statistics on longitudinal evolutions in [125], [126].
Goals: Developing higher order numerical schemes for parallel transport (only low order schemes are available at the moment) and developing variational models to learn the metric or the connections for improving statistical results.

3.1.3. Sparsity in Imaging

3.1.3.1. Inverse problems over measures spaces.

(*Participants:* G. Peyré, V. Duval, C. Poon, Q. Denoyelle) As detailed in Section 2.4 , popular methods for regularizing inverse problems in imaging make use of variational analysis over infinite-dimensional (typically non-reflexive) Banach spaces, such as Radon measures or bounded variation functions.
Our expertise: We have recently shown in [179] how – in the finite dimensional case – the non-smoothness of the functionals at stake is crucial to enforce the emergence of geometrical structures (edges in images or fractures in physical materials [75]) for discrete (finite dimensional) problems. We extended this result in a simple infinite dimensional setting, namely sparse regularization of Radon measures for deconvolution [120]. A deep understanding of those continuous inverse problems is crucial to analyze the behavior of their discrete counterparts, and in [121] we have taken advantage of this understanding to develop a fine analysis of the artifacts induced by discrete (*i.e.* which involve grids) deconvolution models. These works are also closely


Axial

Coronal

Sagittal

Figure 7. Learning Riemannian metrics in diffeomorphic image matching to capture the brain variability: a diagonal operator that encodes the Riemannian metric is learnt on a template brain out of a collection of brain images. The values of the diagonal operator are shown in greyscale. The red curves represent the boundary between white and grey matter. For more details, we refer the reader to [181], which was a first step towards designing effective and robust metric learning algorithms.

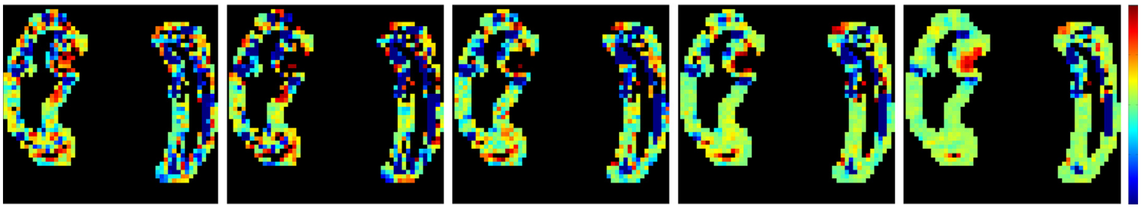


Figure 8. Statistics on initial momenta: In [125], we compared several intersubject transport methodologies to perform statistics on longitudinal evolutions. These longitudinal evolutions are represented by an initial velocity field on the shapes boundaries and these velocity fields are then compared using logistic regression methods that are regularized. The four pictures represent different regularization methods such as L^2, H^1 and regularization including a sparsity prior such as Lasso, Fused Lasso and TV.

related to the problem of limit analysis and yield design in mechanical plasticity, see [100], [75] for an existing collaboration between MOKAPLAN's team members.

Goals: A current major front of research in the mathematical analysis of inverse problems is to extend these results for more complicated infinite dimensional signal and image models, such as for instance the set of piecewise regular functions. The key bottleneck is that, contrary to sparse measures (which are finite sums of Dirac masses), here the objects to recover (smooth edge curves) are not parameterized by a finite number of degrees of freedom. he relevant previous work in this direction are the fundamental results of Chambolle, Caselles and co-workers [59], [52], [108]. They however only deal with the specific case where there is no degradation operator and no noise in the observations. We believe that adapting these approaches using our construction of vanishing derivative pre-certificate [120] could lead to a solution to these theoretical questions.

3.1.3.2. Sub-Riemannian diffusions.

(*Participants:* G. Peyré, J-M. Mirebeau, D. Prandi) Modeling and processing natural images require to take into account their geometry through anisotropic diffusion operators, in order to denoise and enhance directional features such as edges and textures [164], [122]. This requirement is also at the heart of recently proposed models of cortical processing [163]. A mathematical model for these processing is diffusion on sub-Riemanian manifold. These methods assume a fixed, usually linear, mapping from the 2-D image to a lifted function defined on the product of space and orientation (which in turn is equipped with a sub-Riemannian manifold structure).

Our expertise: J-M. Mirebeau is an expert in the discretization of highly anisotropic diffusions through the use of locally adaptive computational stencils [155], [122]. G. Peyré has done several contributions on the definition of geometric wavelets transform and directional texture models, see for instance [164]. Dario Prandi has recently applied methods from sub-Riemannian geometry to image restoration [77].

Goals: A first aspect of this work is to study non-linear, data-adaptive, lifting from the image to the space/orientation domain. This mapping will be implicitly defined as the solution of a convex variational problem. This will open both theoretical questions (existence of a solution and its geometrical properties, when the image to recover is piecewise regular) and numerical ones (how to provide a faithful discretization and fast second order Newton-like solvers). A second aspect of this task is to study the implication of these models for biological vision, in a collaboration with the UNIC Laboratory (directed by Yves Fregnac), located in Gif-sur-Yvette. In particular, the study of the geometry of singular vectors (or "ground states" using the terminology of [70]) of the non-linear sub-Riemannian diffusion operators is highly relevant from a biological modeling point of view.

3.1.3.3. Sparse reconstruction from scanner data.

(*Participants:* G. Peyré, V. Duval, C. Poon) Scanner data acquisition is mathematically modeled as a (sub-sampled) Radon transform [134]. It is a difficult inverse problem because the Radon transform is ill-posed and the set of observations is often aggressively sub-sampled and noisy [172]. Typical approaches [140] try to recovered piecewise smooth solutions in order to recover precisely the position of the organ being imaged. There is however a very poor understanding of the actual performance of these methods, and little is known on how to enhance the recovery.

Our expertise: We have obtained a good understanding of the performance of inverse problem regularization on *compact* domains for pointwise sources localization [120].

Goals: We aim at extending the theoretical performance analysis obtained for sparse measures [120] to the set of piecewise regular 2-D and 3-D functions. Some interesting previous work of C. Poon et al [166] (C. Poon is currently a postdoc in MOKAPLAN) have tackled related questions in the field of variable Fourier sampling for compressed sensing application (which is a toy model for fMRI imaging). These approaches are however not directly applicable to Radon sampling, and require some non-trivial adaptations. We also aim at better exploring the connection of these methods with optimal-transport based fidelity terms such as those introduced in [49].

3.1.3.4. Tumor growth modeling in medical image analysis.

(*Participants:* G. Peyré, F-X. Vialard, J-D. Benamou, L. Chizat) Some applications in medical image analysis require to track shapes whose evolution is governed by a growth process. A typical example is tumor growth, where the evolution depends on some typically unknown but meaningful parameters that need to be estimated. There exist well-established mathematical models [90], [162] of non-linear diffusions that take into account recently biologically observed property of tumors. Some related optimal transport models with mass variations have also recently been proposed [150], which are connected to so-called metamorphoses models in the LDDMM framework [71].

Our expertise: Our team has a strong experience on both dynamical optimal transport models and diffeomorphic matching methods (see Section 3.1.2).

Goals: The close connection between tumor growth models [90], [162] and gradient flows for (possibly non-Euclidean) Wasserstein metrics (see Section 3.1.2) makes the application of the numerical methods we develop particularly appealing to tackle large scale forward tumor evolution simulation. A significant departure from the classical OT-based convex models is however required. The final problem we wish to solve is the backward (inverse) problem of estimating tumor parameters from noisy and partial observations. This also requires to set-up a meaningful and robust data fidelity term, which can be for instance a generalized optimal transport metric.

3.2. Numerical Tools

The above continuous models require a careful discretization, so that the fundamental properties of the models are transferred to the discrete setting. Our team aims at developing innovative discretization schemes as well as associated fast numerical solvers, that can deal with the geometric complexity of the variational problems studied in the applications. This will ensure that the discrete solution is correct and converges to the solution of the continuous model within a guaranteed precision. We give below examples for which a careful mathematical analysis of the continuous to discrete model is essential, and where dedicated non-smooth optimization solvers are required.

3.2.1. Geometric Discretization Schemes

3.2.1.1. Discretizing the cone of convex constraints.

(*Participants:* J-D. Benamou, G. Carlier, J-M. Mirebeau, Q. Mérigot) Optimal transportation models as well as continuous models in economics can be formulated as infinite dimensional convex variational problems with the constraint that the solution belongs to the cone of convex functions. Discretizing this constraint is however a tricky problem, and usual finite element discretizations fail to converge.

Our expertise: Our team is currently investigating new discretizations, see in particular the recent proposal [68] for the Monge-Ampère equation and [154] for general non-linear variational problems. Both offer convergence guarantees and are amenable to fast numerical resolution techniques such as Newton solvers. Since [68] explaining how to treat efficiently and in full generality Transport Boundary Conditions for Monge-Ampère, this is a promising fast and new approach to compute Optimal Transportation viscosity solutions. A monotone scheme is needed. One is based on Froese Oberman work [128], a new different and more accurate approach has been proposed by Mirebeau, Benamou and Collino [66]. As shown in [113], discretizing the constraint for a continuous function to be convex is not trivial. Our group has largely contributed to solve this problem with G. Carlier [104], Quentin Mérigot [157] and J-M. Mirebeau [154]. This problem is connected to the construction of monotone schemes for the Monge-Ampère equation.

Goals: The current available methods are 2-D. They need to be optimized and parallelized. A non-trivial extension to 3-D is necessary for many applications. The notion of c-convexity appears in optimal transport for generalized displacement costs. How to construct an adapted discretization with “good” numerical properties is however an open problem.

3.2.1.2. Numerical JKO gradient flows.

(*Participants:* J-D. Benamou, G. Carlier, J-M. Mirebeau, G. Peyré, Q. Mérigot) As detailed in Section 2.3 , gradient Flows for the Wasserstein metric (aka JKO gradient flows [137]) provides a variational formulation of many non-linear diffusion equations. They also open the way to novel discretization schemes. From a computational point, although the JKO scheme is constructive (it is based on the implicit Euler scheme), it has not been very much used in practice numerically because the Wasserstein term is difficult to handle (except in dimension one).
Our expertise:

Solving one step of a JKO gradient flow is similar to solving an Optimal transport problem. A geometrical a discretization of the Monge-Ampère operator approach has been proposed by Mérigot, Carlier, Oudet and Benamou in [65] see Figure 4 . The Gamma convergence of the discretisation (in space) has been proved.
Goals: We are also investigating the application of other numerical approaches to Optimal Transport to JKO gradient flows either based on the CFD formulation or on the entropic regularization of the Monge-Kantorovich problem (see section 3.2.3). An in-depth study and comparison of all these methods will be necessary.

3.2.2. Sparse Discretization and Optimization

3.2.2.1. From discrete to continuous sparse regularization and transport.

(*Participants:* V. Duval, G. Peyré, G. Carlier, Jalal Fadili (ENSICaen), Jérôme Malick (CNRS, Univ. Grenoble)) While pervasive in the numerical analysis community, the problem of discretization and Γ-convergence from discrete to continuous is surprisingly over-looked in imaging sciences. To the best of our knowledge, our recent work [120], [121] is the first to give a rigorous answer to the transition from discrete to continuous in the case of the spike deconvolution problem. Similar problems of Γ-convergence are progressively being investigated in the optimal transport community, see in particular [105].
Our expertise: We have provided the first results on the discrete-to-continous convergence in both sparse regularization variational problems [120], [121] and the static formulation of OT and Wasserstein barycenters [105]
Goals: In a collaboration with Jérôme Malick (Inria Grenoble), our first goal is to generalized the result of [120] to generic partly-smooth convex regularizers routinely used in imaging science and machine learning, a prototypal example being the nuclear norm (see [179] for a review of this class of functionals). Our second goal is to extend the results of [105] to the novel class of entropic discretization schemes we have proposed [64], to lay out the theoretical foundation of these ground-breaking numerical schemes.

3.2.2.2. Polynomial optimization for grid-free regularization.

(*Participants:* G. Peyré, V. Duval, C. Poon) There has been a recent spark of attention of the imaging community on so-called “grid free” methods, where one tries to directly tackle the infinite dimensional recovery problem over the space of measures, see for instance [96], [120]. The general idea is that if the range of the imaging operator is finite dimensional, the associated dual optimization problem is also finite dimensional (for deconvolution, it corresponds to optimization over the set of trigonometric polynomials).
Our expertise: We have provided in [120] a sharp analysis of the support recovery property of this class of methods for the case of sparse spikes deconvolution.
Goals: A key bottleneck of these approaches is that, while being finite dimensional, the dual problem necessitates to handle a constraint of polynomial positivity, which is notoriously difficult to manipulate (except in the very particular case of 1-D problems, which is the one exposed in [96]). A possible, but very costly, methodology is to ressort to Lasserre’s SDP representation hierarchy [142]. We will make use of these approaches and study how restricting the level of the hierarchy (to obtain fast algorithms) impacts the recovery performances (since this corresponds to only computing approximate solutions). We will pay a particular attention to the recovery of 2-D piecewise constant functions (the so-called total variation of functions regularization [171]), see Figure 3 for some illustrative applications of this method.

3.2.3. First Order Proximal Schemes

3.2.3.1. L^2 proximal methods.

(*Participants:* G. Peyré, J-D. Benamou, G. Carlier, Jalal Fadili (ENSICaen)) Both sparse regularization problems in imaging (see Section 2.4) and dynamical optimal transport (see Section 2.3) are instances of large scale, highly structured, non-smooth convex optimization problems. First order proximal splitting optimization algorithms have recently gained lots of interest for these applications because they are the only ones capable of scaling to giga-pixel discretizations of images and volumes and at the same time handling non-smooth objective functions. They have been successfully applied to optimal transport [60], [158], congested optimal transport [89] and to sparse regularizations (see for instance [168] and the references therein).

Our expertise: The pioneering work of our team has shown how these proximal solvers can be used to tackle the dynamical optimal transport problem [60], see also [158]. We have also recently developed new proximal schemes that can cope with non-smooth composite objectives functions [168].

Goals: We aim at extending these solvers to a wider class of variational problems, most notably optimization under divergence constraints [62]. Another subject we are investigating is the extension of these solvers to both non-smooth and non-convex objective functionals, which are mandatory to handle more general transportation problems and novel imaging regularization penalties.

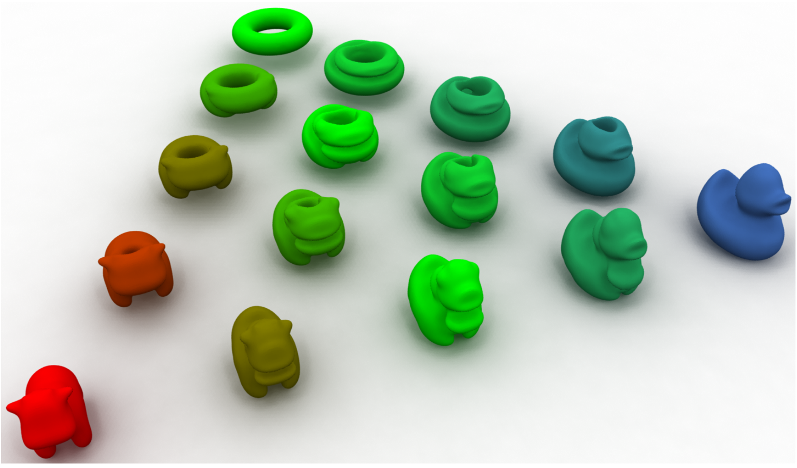


Figure 9. Example of barycenter between shapes computed using optimal transport barycenters of the uniform densities inside the 3 extremal shapes, computed as detailed in [176]. Note that the barycenters are not in general uniform distributions, and we display them as the surface defined by a suitable level-set of the density.

3.2.3.2. Bregman proximal methods.

(*Participants:* G. Peyré G. Carlier, L. Nenna, J-D. Benamou, L. Nenna, Marco Cuturi (Kyoto Univ.)) The entropic regularization of the Kantorovich linear program for OT has been shown to be surprisingly simple and efficient, in particular for applications in machine learning [118]. As shown in [64], this is a special instance of the general method of Bregman iterations, which is also a particular instance of first order proximal schemes according to the Kullback-Leibler divergence.

Our expertise: We have recently [64] shown how Bregman projections [80] and Dykstra algorithm [56] offer a generic optimization framework to solve a variety of generalized OT problems. Carlier and Dupuis [101] have designed a new method based on alternate Dykstra projections and applied it to the *principal-agent problem* in microeconomics. We have applied this method in computer graphics in a paper accepted in SIGGRAPH 2015 [176]. Figure 9 shows the potential of our approach to handle giga-voxel datasets: the input volumetric densities are discretized on a 100^3 computational grid.
Goals: Following some recent works (see in particular [110]) we first aim at studying primal-dual optimization schemes according to Bregman divergences (that would go much beyond gradient descent and iterative projections), in order to offer a versatile and very effective framework to solve variational problems involving OT terms. We then also aim at extending the scope of usage of this method to applications in quantum mechanics (Density Functional Theory, see [114]) and fluid dynamics (Brenier's weak solutions of the incompressible Euler equation, see [81]). The computational challenge is that realistic physical examples are of a huge size not only because of the space discretization of one marginal but also because of the large number of marginals involved (for incompressible Euler the number of marginals equals the number of time steps).

NACHOS Project-Team

3. Research Program

3.1. Scientific foundations

The research activities undertaken by the team aim at developing innovative numerical methodologies putting the emphasis on several features:

- **Accuracy**. The foreseen numerical methods should rely on discretization techniques that best fit to the geometrical characteristics of the problems at hand. Methods based on unstructured, locally refined, even non-conforming, simplicial meshes are particularly attractive in this regard. In addition, the proposed numerical methods should also be capable to accurately describe the underlying physical phenomena that may involve highly variable space and time scales. Both objectives are generally addressed by studying so-called hp-adaptive solution strategies which combine h-adaptivity using local refinement/coarsening of the mesh and p-adaptivity using adaptive local variation of the interpolation order for approximating the solution variables. However, for physical problems involving strongly heterogeneous or high contrast propagation media, such a solution strategy may not be sufficient. Then, for dealing accurately with these situations, one has to design numerical methods that specifically address the multiscale nature of the underlying physical phenomena.
- **Numerical efficiency**. The simulation of unsteady problems most often relies on explicit time integration schemes. Such schemes are constrained by a stability criterion, linking some space and time discretization parameters, that can be very restrictive when the underlying mesh is highly non-uniform (especially for locally refined meshes). For realistic 3D problems, this can represent a severe limitation with regards to the overall computing time. One possible overcoming solution consists in resorting to an implicit time scheme in regions of the computational domain where the underlying mesh size is very small, while an explicit time scheme is applied elsewhere in the computational domain. The resulting hybrid explicit-implicit time integration strategy raises several challenging questions concerning both the mathematical analysis (stability and accuracy, especially for what concern numerical dispersion), and the computer implementation on modern high performance systems (data structures, parallel computing aspects). A second, often considered approach is to devise a local time stepping strategy. Beside, when considering time-harmonic (frequency-domain) wave propagation problems, numerical efficiency is mainly linked to the solution of the system of algebraic equations resulting from the discretization in space of the underlying PDE model. Various strategies exist ranging from the more robust and efficient sparse direct solvers to the more flexible and cheaper (in terms of memory resources) iterative methods. Current trends tend to show that the ideal candidate will be a judicious mix of both approaches by relying on domain decomposition principles.
- **Computational efficiency**. Realistic 3D wave propagation problems involve the processing of very large volumes of data. The latter results from two combined parameters: the size of the mesh i.e the number of mesh elements, and the number of degrees of freedom per mesh element which is itself linked to the degree of interpolation and to the number of physical variables (for systems of partial differential equations). Hence, numerical methods must be adapted to the characteristics of modern parallel computing platforms taking into account their hierarchical nature (e.g multiple processors and multiple core systems with complex cache and memory hierarchies). In addition, appropriate parallelization strategies need to be designed that combine SIMD and MIMD programming paradigms.

From the methodological point of view, the research activities of the team are concerned with four main topics: (1) high order finite element type methods on unstructured or hybrid structured/unstructured meshes for the discretization of the considered systems of PDEs, (2) efficient time integration strategies for dealing with grid induced stiffness when using non-uniform (locally refined) meshes, (3) numerical treatment of complex propagation media models (e.g. physical dispersion models), (4) algorithmic adaptation to modern high performance computing platforms.

3.2. High order discretization methods

3.2.1. The Discontinuous Galerkin method

The Discontinuous Galerkin method (DG) was introduced in 1973 by Reed and Hill to solve the neutron transport equation. From this time to the 90's a review on the DG methods would likely fit into one page. In the meantime, the Finite Volume approach (FV) has been widely adopted by computational fluid dynamics scientists and has now nearly supplanted classical finite difference and finite element methods in solving problems of non-linear convection and conservation law systems. The success of the FV method is due to its ability to capture discontinuous solutions which may occur when solving non-linear equations or more simply, when convecting discontinuous initial data in the linear case. Let us first remark that DG methods share with FV methods this property since a first order FV scheme may be viewed as a 0th order DG scheme. However a DG method may also be considered as a Finite Element (FE) one where the continuity constraint at an element interface is released. While keeping almost all the advantages of the FE method (large spectrum of applications, complex geometries, etc.), the DG method has other nice properties which explain the renewed interest it gains in various domains in scientific computing as witnessed by books or special issues of journals dedicated to this method [41]- [42]- [43]- [48]:

- It is naturally adapted to a high order approximation of the unknown field. Moreover, one may increase the degree of the approximation in the whole mesh as easily as for spectral methods but, with a DG method, this can also be done very locally. In most cases, the approximation relies on a polynomial interpolation method but the DG method also offers the flexibility of applying local approximation strategies that best fit to the intrinsic features of the modeled physical phenomena.
- When the space discretization is coupled to an explicit time integration scheme, the DG method leads to a block diagonal mass matrix whatever the form of the local approximation (e.g. the type of polynomial interpolation). This is a striking difference with classical, continuous FE formulations. Moreover, the mass matrix may be diagonal if the basis functions are orthogonal.
- It easily handles complex meshes. The grid may be a classical conforming FE mesh, a non-conforming one or even a hybrid mesh made of various elements (tetrahedra, prisms, hexahedra, etc.). The DG method has been proven to work well with highly locally refined meshes. This property makes the DG method more suitable (and flexible) to the design of some hp-adaptive solution strategy.
- It is also flexible with regards to the choice of the time stepping scheme. One may combine the DG spatial discretization with any global or local explicit time integration scheme, or even implicit, provided the resulting scheme is stable.
- It is naturally adapted to parallel computing. As long as an explicit time integration scheme is used, the DG method is easily parallelized. Moreover, the compact nature of DG discretization schemes is in favor of high computation to communication ratio especially when the interpolation order is increased.

As with standard FE methods, a DG method relies on a variational formulation of the continuous problem at hand. However, due to the discontinuity of the global approximation, this variational formulation has to be defined locally, at the element level. Then, a degree of freedom in the design of a DG method stems from the approximation of the boundary integral term resulting from the application of an integration by parts to the element-wise variational form. In the spirit of FV methods, the approximation of this boundary integral term calls for a numerical flux function which can be based on either a centered scheme or an upwind scheme, or a blending between these two schemes.

3.2.2. High order DG methods for wave propagation models

DG methods are at the heart of the activities of the team regarding the development of high order discretization schemes for the PDE systems modeling electromagnetic and elatsodynamic wave propagation.

- **Nodal DG methods for time-domain problems**. For the numerical solution of the time-domain Maxwell equations, we have first proposed a non-dissipative high order DGTD (Discontinuous Galerkin Time-Domain) method working on unstructured conforming simplicial meshes [13]. This DG method combines a central numerical flux function for the approximation of the integral term at the interface of two neighboring elements with a second order leap-frog time integration scheme. Moreover, the local approximation of the electromagnetic field relies on a nodal (Lagrange type) polynomial interpolation method. Recent achievements by the team deal with the extension of these methods towards non-conforming unstructured [10]-[11] and hybrid structured/unstructured meshes [6], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [4]-[19]-[18]. A high order DG method has also been proposed for the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [2]-[9].
- **Hybridizable DG (HDG) method for time-domain and time-harmonic problems**. For the numerical treatment of the time-harmonic Maxwell equations, nodal DG methods can also be considered [8]. However, such DG formulations are highly expensive, especially for the discretization of 3D problems, because they lead to a large sparse and undefinite linear system of equations coupling all the degrees of freedom of the unknown physical fields. Different attempts have been made in the recent past to improve this situation and one promising strategy has been recently proposed by Cockburn *et al.*[46] in the form of so-called hybridizable DG formulations. The distinctive feature of these methods is that the only globally coupled degrees of freedom are those of an approximation of the solution defined only on the boundaries of the elements. This work is concerned with the study of such Hybridizable Discontinuous Galerkin (HDG) methods for the solution of the system of Maxwell equations in the time-domain when the time integration relies on an implicit scheme, or in the frequency-domain. The team has been a precursor in the development of HDG methods for the frequency-domain Maxwell equations [15]-[16].
- **Multiscale DG methods for time-domain problems**. More recently, in collaboration with LNCC in Petropolis (Frédéric Valentin) the framework of the HOMAR assoacite team, we are investigating a family of methods specifically designed for an accurate and efficient numerical treatment of multiscale wave propagation problems. These methods, referred to as Multiscale Hybrid Mixed (MHM) methods, are currently studied in the team for both time-domain electromagnetic and elastodynamic PDE models. They consist in reformulating the mixed variational form of each system into a global (arbitrarily coarse) problem related to a weak formulation of the boundary condition (carried by a Lagrange multiplier that represents e.g. the normal stress tensor in elastodynamic sytems), and a series of small, element-wise, fully decoupled problems resembling to the initial one and related to some well chosen partition of the solution variables on each element. By construction, that methodology is fully parallelizable and recursivity may be used in each local problem as well, making MHM methods belonging to multi-level highly parallelizable methods. Each local problem may be solved using DG or classical Galerkin FE approximations combined with some appropriate time integration scheme (θ-scheme or leap-frog scheme).

3.3. Efficient time integration strategies

The use of unstructured meshes (based on triangles in two space dimensions and tetrahedra in three space dimensions) is an important feature of the DGTD methods developed in the team which can thus easily deal with complex geometries and heterogeneous propagation media. Moreover, DG discretization methods are naturally adapted to local, conforming as well as non-conforming, refinement of the underlying mesh. Most of the existing DGTD methods rely on explicit time integration schemes and lead to block diagonal mass matrices which is often recognized as one of the main advantages with regards to continuous finite element methods.

However, explicit DGTD methods are also constrained by a stability condition that can be very restrictive on highly refined meshes and when the local approximation relies on high order polynomial interpolation. There are basically three strategies that can be considered to cure this computational efficiency problem. The first approach is to use an unconditionally stable implicit time integration scheme to overcome the restrictive constraint on the time step for locally refined meshes. In a second approach, a local time stepping strategy is combined with an explicit time integration scheme. In the third approach, the time step size restriction is overcome by using a hybrid explicit-implicit procedure. In this case, one blends a time implicit and a time explicit schemes where only the solution variables defined on the smallest elements are treated implicitly. The first and third options are considered in the team in the framework of DG [4]-[19]-[18] and HDG discretization methods.

3.4. Numerical treatment of complex material models

Towards the general aim of being able to consider concrete physical situations, we are interested in taking into account in the numerical methodologies that we study, a better description of the propagation of waves in realistic media. In the case of electromagnetics, a typical physical phenomenon that one has to consider is *dispersion*. It is present in almost all media and expresses the way the material reacts to an electromagnetic field. In the presence of an electric field a medium does not react instantaneously and thus presents an electric polarization of the molecules or electrons that itself influences the electric displacement. In the case of a linear homogeneous isotropic media, there is a linear relation between the applied electric field and the polarization. However, above some range of frequencies (depending on the considered material), the dispersion phenomenon cannot be neglected and the relation between the polarization and the applied electric field becomes complex. This is rendered via a frequency-dependent complex permittivity. Several models of complex permittivity exist. Concerning biological media, the Debye model is commonly adopted in the presence of water, biological tissues and polymers, so that it already covers a wide range of applications [14]. In the context of nanoplasmonics, one is interested in modeling the dispersion effects on metals on the nanometer scale and at optical frequencies. In this case, the Drude or the Drude-Lorentz models are generally chosen [21]. In the context of seismic wave propagation, we are interested by the intrinsic attenuation of the medium [20]. In realistic configurations, for instance in sedimentary basins where the waves are trapped, we can observe site effects due to local geological and geotechnical conditions which result in a strong increase in amplification and duration of the ground motion at some particular locations. During the wave propagation in such media, a part of the seismic energy is dissipated because of anelastic losses relied to the internal friction of the medium. For these reasons, numerical simulations based on the basic assumption of linear elasticity are no more valid since this assumption results in a severe overestimation of amplitude and duration of the ground motion, even when we are not in presence of a site effect, since intrinsic attenuation is not taken into account.

3.5. High performance numerical computing

Beside basic research activities related to the design of numerical methods and resolution algorithms for the wave propagation models at hand, the team is also committed to demonstrate the benefits of the proposed numerical methodologies in the simulation of challenging three-dimensional problems pertaining to computational electromagnetics and computational geoseismics. For such applications, parallel computing is a mandatory path. Nowadays, modern parallel computers most often take the form of clusters of heterogeneous multiprocessor systems, combining multiple core CPUs with accelerator cards (e.g Graphical Processing Units - GPUs), with complex hierarchical distributed-shared memory systems. Developing numerical algorithms that efficiently exploit such high performance computing architectures raises several challenges, especially in the context of a massive parallelism. In this context, current efforts of the team are towards the exploitation of multiple levels of parallelism (computing systems combining CPUs and GPUs) through the study of hierarchical SPMD (Single Program Multiple Data) strategies for the parallelization of unstructured mesh based solvers.

NANO-D Project-Team

3. Research Program

3.1. The need for practical design of nanosystems

Computing has long been an essential tool of engineering. During the twentieth century, the development of macroscopic engineering has been largely stimulated by progress in numerical design and prototyping. Cars, planes, boats, and many other manufactured objects are nowadays, for the most part, designed and tested on computers. Digital prototypes have progressively replaced actual ones, and effective computer-aided engineering tools (e.g., CATIA, SolidWorks, T-FLEX CAD, Alibre Design, TopSolid, etc.) have helped cut costs and reduce production cycles of macroscopic systems [66].

The twenty-first century is most likely to see a similar development at the atomic scale. Indeed, the recent years have seen tremendous progress in nanotechnology. The magazine Science, for example, recently featured a paper demonstrating an example of DNA nanotechnology, where DNA strands are stacked together through programmable self-assembly [35]. In February 2007, the cover of Nature Nanotechnology showed a "nano-wheel" composed of a few atoms only. Several nanosystems have already been demonstrated, including a *de-novo* computationally designed protein interface [37], a wheelbarrow molecule [44], a nano-car [70], a Morse molecule [18], etc. Typically, these designs are optimized using semi-empirical quantum mechanics calculations, such as the semi-empirical ASED+ calculation technique [19].

While impressive, these are but two examples of the nanoscience revolution already impacting numerous fields, including electronics and semiconductors [53], textiles [52], [40], energy [55], food [29], drug delivery [39], [72], chemicals [41], materials [30], the automotive industry [16], aerospace and defense [38], medical devices and therapeutics [33], medical diagnostics [73], etc. According to some estimates, the world market for nanotechnology-related products and services will reach one trillion dollars by 2015 [65]. Nano-engineering groups are multiplying throughout the world, both in academia and in the industry: in the USA, the MIT has a "NanoEngineering" research group, Sandia National Laboratories created a "National Institute for Nano Engineering", to name a few; China founded a "National Center for Nano Engineering" in 2003, etc. Europe is also a significant force in public funding of nanoscience and nanotechnology and, in Europe, Grenoble and the Rhone-Alpes area gather numerous institutions and organizations related to nanoscience.

Of course, not all small systems that currently fall under the label "nano" have mechanical, electronic, optical properties similar to the examples given above. Furthermore, current construction capabilities lack behind some of the theoretical designs which have been proposed, such as the planetary gear designed by Eric Drexler at Nanorex. However, the trend is clearly for adding more and more functionality to nanosystems. While designing nanosystems is still very much an art mostly performed by physicists, chemists and biologists in labs throughout the world, there is absolutely no doubt that fundamental engineering practices will progressively emerge, and that these practices will be turned into quantitative rules and methods. Similar to what has happened with macroscopic engineering, powerful and generic software will then be employed to engineer complex nanosystems.

3.2. Challenges of practical nanosystem design

As with macrosystems, designing nanosystems will involve modeling and simulation within software applications: modeling, especially structural modeling, will be concerned with the creation of potentially complex chemical structures such as the examples above, using a graphical user interface, parsers, scripts, builders, etc.; simulation will be employed to predict some properties of the constructed models, including mechanical properties, electronic properties, chemical properties, etc.

In general, design may be considered as an “inverse simulation problem”. Indeed, designed systems often need to be optimized so that their properties — predicted by simulation — satisfy specific objectives and constraints (e.g. a car should have a low drag coefficient, a drug should have a high affinity and selectivity to a target protein, a nano-wheel should roll when pushed, etc.). Being the main technique employed to predict properties, simulation is essential to the design process. At the nanoscale, simulation is even more important. Indeed, physics significantly constrains atomic structures (e.g. arbitrary inter-atomic distances cannot exist), so that a tentative atomic shape should be checked for plausibility much earlier in the design process (e.g. remove atomic clashes, prevent unrealistic, high-energy configurations, etc.). For nanosystems, thus, efficient simulation algorithms are required both when modeling structures and when predicting systems properties. Precisely, an effective software tool to design nanosystems should (a) allow for interactive physically-based modeling, where all user actions (e.g. displacing atoms, modifying the system’s topology, etc.) are automatically followed by a few steps of energy minimization to help the user build plausible structures, even for large number of atoms, and (b) be able to predict systems properties, through a series of increasingly complex simulations.

3.3. Current simulation approaches

Even though the growing need for effective nanosystem design will still increase the demand for simulation, a lot of research has already gone into the development of efficient simulation algorithms. Typically, two approaches are used: (a) increasing the computational resources (use super-computers, computer clusters, grids, develop parallel computing approaches, etc.), or (b) simulating simplified physics and/or models. Even though the first strategy is sometimes favored, it is expensive and, it could be argued, inefficient: only a few supercomputers exist, not everyone is willing to share idle time from their personal computer, etc. Surely, we would see much less creativity in cars, planes, and manufactured objects all around if they had to be designed on one of these scarce super-resources.

The second strategy has received a lot of attention. Typical approaches to speed up molecular mechanics simulation include lattice simulations [75], removing some degrees of freedom (e.g. keeping torsion angles only [51], [71]), coarse-graining [74], [68], [20], [69], multiple time step methods [61], [62], fast multipole methods [34], parallelization [46], averaging [28], multi-scale modeling [27], [24], reactive force fields [26], [78], interactive multiplayer games for predicting protein structures [32], etc. Until recently, quantum mechanics methods, as well as mixed quantum / molecular mechanics methods were still extremely slow. One breakthrough has consisted in the discovery of linear-scaling, divide-and-conquer quantum mechanics methods [76], [77].

Overall, the computational community has already produced a variety of sophisticated simulation packages, for both classical and quantum simulation: ABINIT, AMBER, CHARMM, Desmond, GROMOS and GROMACS, LAMMPS, NAMD, ROSETTA, SIESTA, TINKER, VASP, YASARA, etc. Some of these tools are open source, while some others are available commercially, sometimes via integrating applications: Ascalaph Designer, BOSS, Discovery Studio, Materials Studio, Maestro, MedeA, MOE, NanoEngineer-1, Spartan, etc. Other tools are mostly concerned with visualization, but may sometimes be connected to simulation packages: Avogadro, PyMol, VMD, Zodiac, etc. The nanoHUB network also includes a rich set of tools related to computational nanoscience.

To the best of our knowledge, however, all methods which attempt to speed up dynamics simulations perform a priori simplification assumptions, which might bias the study of the simulated phenomenon. A few recent, interesting approaches have managed to combine several levels of description (e.g. atomistic and coarse-grained) into a single simulation, and have molecules switch between levels during simulation, including the adaptive resolution method [57], [58], [59], [60], the adaptive multiscale method [54], and the adaptive partitioning of the Lagrangian method [42]. Although these approaches have demonstrated some convincing applications, they all suffer from a number of limitations stemming from the fact that they are either ad hoc methods tuned to fix specific problems (e.g. fix density problems in regions where the level of description changes), or mathematically founded methods that necessitate to “calibrate” potentials so that they can be mixed (i.e. all potentials have to agree on a reference point). In general, multi-scale methods, even when they do not allow molecules to switch between levels of detail during simulation, have to solve the problem of rigorously combining multiple levels of description (i.e. preserve statistics, etc.), of assigning appropriate levels to different parts of the simulated system ("simplify as much as possible, but not too much"), and of determining computable mappings between levels of description (especially, adding back detail when going from coarse-grained descriptions to fine-grained descriptions).

3.4. Research axes

The goal of the NANO-D group is to help current and future designers of *nanosystems*, i.e. systems studied or designed at the atomic scale (whether natural or artificial, independently of the application domain, including structural biology, material science, chemistry, etc.) by developing the **foundations of a software application which will run on a desktop computer, and will allow for efficient analysis, design, modeling and simulation of nanosystems**.

To achieve this, we will be developing a series of **adaptive methods and algorithms** that allow users to focus computational resources on the parts of the models that they want to simulate, and that allow to finely trade between speed and precision.

In parallel, we will develop the architecture of a new desktop application for virtual prototyping of nanosystems, and will integrate all our algorithms into this application. Furthermore, the architecture of this platform will be open, so that independent developers may add modules, for **multiple application domains** (physics, biology, chemistry, materials, electronics, etc.). With this open platform, we will attempt to federate the research performed in computational nanoscience throughout the world.

This application is called **SAMSON: "Software for Adaptive Modeling and Simulation Of Nanosystems"**.

Our two research axes are:

1. **Developing adaptive algorithms for simulating nanosystems**
   - **Defining adaptive Hamiltonians**: In order to be able to perform simulations with good mathematical properties, we are expanding on our recent work on *adaptively restrained Hamiltonians*[22], *i.e.* modified Hamiltonian representations of molecular systems that are able to switch degrees of freedom on and off during a simulation. These will allow us to finely trade between precision and computational performance, by choosing arbitrarily the number of degrees of freedom. Even though we have already obtained some promising results in this domain, our goal is to develop several different simplification methods.
   - **Developing algorithms for incremental potential update**: In order to benefit from performing adaptive particle simulations, we need to develop a series of algorithms that will take advantage of the fact that some (potentially relative) atomic positions are frozen. We have already demonstrated how this is possible for torsion-angle quasi-static simulation of classical bio-molecular force-fields [67], for neighbor search between large rigid molecules [21], and for bond-order reactive force-fields [25]. We are developing new algorithms for incremental neighbor search, energy and force updates corresponding to the adaptive Hamiltonians that we are defining.
2. **Developing algorithms for modeling molecular interactions**
   - **Developing knowledge-driven methods, potentials and algorithms**: Over time, more and more experimental information becomes available. One can use this information to predict and discover new types of molecular interactions and various mechanisms or molecular organization. For example, currently there are more than 50,000 protein structures of a high resolution stored in the Protein Data Bank [23] and over 500,000 structures of small molecules stored in the Cambridge Structural Database [17]. We are developing algorithms for protein-protein interactions and protein-ligand interactions.

- **Developing parametrization algorithms for interaction potentials**: Molecular models typically require their own potential energy function (or a *forcefield*) to be assigned. However, the development of a new potential function is a very difficult and sometimes challenging task [43]. Therefore, we are developing algorithms for automatic parametrization of new potential functions for some particular representations of a molecular system.
- **Developing algorithms for exhaustive sampling**: Some application domains, such as computational docking, cryo-EM rigid-body fitting, etc., require sampling in a low-dimensional space. For such applications it is advantageous to perform an exhaustive search rather than accelerated sampling [64]. Therefore, we are developing fast search methods to perform exhaustive search.

NECS Project-Team

3. Research Program

3.1. Introduction

NECS team deals with Networked Control Systems. Since its foundation in 2007, the team has been addressing issues of control under imperfections and constraints deriving from the network (limited computation resources of the embedded systems, delays and errors due to communication, limited energy resources), proposing co-design strategies. The team has recently moved its focus towards general problems on *control of network systems*, which involve the analysis and control of dynamical systems with a network structure or whose operation is supported by networks. This is a research domain with substantial growth and is now recognized as a priority sector by the IEEE Control Systems Society: IEEE has started a new journal, IEEE Transactions on Control of Network Systems, whose first issue appeared in 2014.

More in detail, the research program of NECS team is along lines described in the following sections.

3.2. Distributed estimation and data fusion in network systems

This research topic concerns distributed data combination from multiple sources (sensors) and related information fusion, to achieve more specific inference than could be achieved by using a single source (sensor). It plays an essential role in many networked applications, such as communication, networked control, monitoring, and surveillance. Distributed estimation has already been considered in the team. We wish to capitalize and strengthen these activities by focusing on integration of heterogeneous, multidimensional, and large data sets:

- Heterogeneity and large data sets. This issue constitutes a clearly identified challenge for the future. Indeed, heterogeneity comes from the fact that data are given in many forms, refer to different scales, and carry different information. Therefore, data fusion and integration will be achieved by developing new multi-perception mathematical models that can allow tracking continuous (macroscopic) and discrete (microscopic) dynamics under a unified framework while making different scales interact with each other. More precisely, many scales are considered at the same time, and they evolve following a unique fully-integrated dynamics generated by the interactions of the scales. The new multi-perception models will be integrated to forecast, estimate and broadcast useful system states in a distributed way. Targeted applications include traffic networks and navigation, and concern recent grant proposals that team has elaborated, among which the SPEEDD EU FP7 project, which has started in February 2014.
- Multidimensionality. This issue concerns the analysis and the processing of multidimensional data, organized in multiway array, in a distributed way. Robustness of previously-developed algorithms will be studied. In particular, the issue of missing data will be taken into account. In addition, since the considered multidimensional data are generated by dynamic systems, dynamic analysis of multiway array (or tensors) will be considered. The targeted applications concern distributed detection in complex networks and distributed signal processing for collaborative networks. This topic is developed in strong collaboration with UFC (Brazil).

3.3. Network systems and graph analysis

This is a research topic at the boundaries between graph theory and dynamical systems theory.

A first main line of research will be to study complex systems whose interactions are modeled with graphs, and to unveil the effect of the graph topology on system-theoretic properties such as observability or controllability. In particular, on-going work concerns observability of graph-based systems: after preliminary results concerning consensus systems over distance-regular graphs, the aim is to extend results to more general networks. A special focus will be on the notion of ‘generic properties’, namely properties which depend only on the underlying graph describing the sparsity pattern, and hold true almost surely with a random choice of the non-zero coefficients. Further work will be to explore situations in which there is the need for new notions different from the classical observability or controllability. For example, in opinion-forming in social networks or in formation of birds flocks, the potential leader might have a goal different from classical controllability. On the one hand, his goal might be much less ambitious than the classical one of driving the system to any possible state (e.g., he might want to drive everybody near its own opinion, only, and not to any combination of different individual opinions), and on the other hand he might have much weaker tools to construct his control input (e.g., he might not know the whole system’s dynamics, but only some local partial information). Another example is the question of detectability of an unknown input under the assumption that such an input has a sparsity constraint, a question arising from the fact that a cyber-physical attack might be modeled as an input aiming at controlling the system’s state, and that limitations in the capabilities of the attacker might be modeled as a sparsity constraint on the input.

A second line of research will concern graph discovery, namely algorithms aiming at reconstructing some properties of the graph (such as the number of vertices, the diameter, the degree distribution, or spectral properties such as the eigenvalues of the graph Laplacian), using some measurements of quantities related to a dynamical system associated with the graph. It will be particularly challenging to consider directed graphs, and to impose that the algorithm is anonymous, i.e., that it does not makes use of labels identifying the different agents associated with vertices.

3.4. Collaborative and distributed network control

This research line deals with the problem of designing controllers with a limited use of the network information (i.e. with restricted feedback), and with the aim to reach a pre-specified global behavior. This is in contrast to centralized controllers that use the whole system information and compute the control law at some central node. Collaborative control has already been explored in the team in connection with the underwater robot fleet, and to some extent with the source seeking problem. It remains however a certain number of challenging problems that the team wishes to address:

- Design of control with limited information, able to lead to desired global behaviors. Here the graph structure is imposed by the problem, and we aim to design the “best” possible control under such a graph constraint [0]. The team would like to explore further this research line, targeting a better understanding of possible metrics to be used as a target for optimal control design. In particular, and in connection with the traffic application, the long-standing open problem of ramp metering control under minimum information will be addressed.
- Clustering control for large networks. For large and complex systems composed of several sub-networks, feedback design is usually treated at the sub-network level, and most of the times without taking into account natural interconnections between sub-networks. The team is exploring new control strategies, exploiting the emergent behaviors resulting from new interconnections between the network components. This requires first to build network models operating in aggregated clusters, and then to re-formulate problems where the control can be designed using the cluster boundaries rather than individual control loops inside of each network. Examples can be found in the transportation application domain, where a significant challenge will be to obtain dynamic partitioning and clustering of heterogeneous networks in homogeneous sub-networks, and then to control the perimeter flows of the clusters to optimize the network operation. This topic is at the core of the Advanced ERC project Scale-FreeBack.

[0] Such a problem has been previously addressed in some specific applications, particularly robot fleets, and only few recent theoretical works have initiated a more systematic system-theoretic study of sparsity-constrained system realization theory and of sparsity-constrained feedback control.

3.5. Transportation networks

This is currently the main application domain of the NECS team. Several interesting problems in this area capture many of the generic networks problems described above. For example, distributed collaborative algorithms can be devised for ramp-metering control and traffic-density balancing can be achieved using consensus concepts. The team is already strongly involved in this field, both this theoretical works on traffic modeling, prediction and control, and with the Grenoble Traffic Lab platform. These activities will be continued and strengthened, also thanks to the contributions from the new staff member M.L. Delle Monache.

NON-A Project-Team

3. Research Program

3.1. General annihilators

Estimation is quite easy in the absence of perturbations. It becomes challenging in more realistic situations, faced to measurement noises or other unknown inputs. In our works, as well as in the founding text of *Non-A*, we have shown how our estimation techniques can successfully get rid of perturbations of the so-called *structured* type, which means the ones that can be annihilated by some linear differential operator (called the annihilator). *ALIEN* already defined such operators by integral operators, but using more general convolution operators is an alternative to be analyzed, as well as defining the "best way to kill" perturbations. Open questions are:

OQ1) Does a normal form exist for such annihilators?

OQ2) Or, at least, does there exist an adequate basis representation of the annihilator in some adequate algebra?

OQ3) And lastly, can the annihilator parameters be derived from efficient tuning rules?

The two first questions will directly impact Indicators 1 (time) and 2 (complexity), whereas the last one will impact indicator 3 (robustness).

3.2. Numerical differentiation

Estimating the derivative of a (noisy) signal with a sufficient accuracy can be seen as a key problem in domains of control and diagnosis, as well as signal and image processing. At the present stage of our research, the estimation of the n-th order time derivatives of noisy signals (including noise filtering for $n = 0$) appears as a common area for the whole project, either as a research field, or as a tool that is used both for model-based and model-free techniques. *One of the open questions is about the robustness issues (Indicator 3) with respect to the annihilator, the parameters and the numerical implementation choices.*

Two classes of techniques are considered here (**Model-based** and **Model-free**), both of them aiming at non-asymptotic estimation.

In what we call *model-based techniques*, the derivative estimation is regarded as an observation problem, which means the software-based reconstruction of unmeasured variables and, more generally, a left inversion problem [0]. This involves linear/homogeneous/nonlinear state models, including ordinary equations, systems with delays, hybrid systems with impulses or switches [0], which still has to be exploited in the finite-time and fixed-time context. Power electronics is already one of the possible applications.

Model-free techniques concern the works initiated by *ALIEN*, which rely on the only information contained in the output signal and its derivatives. The corresponding algorithms rely on our algebraic annihilation viewpoint. *One open question is: How to provide an objective comparison analysis between Model-based and Model-free estimation techniques? For this, we will only concentrate on Non-Asymptotic ones. This comparison will have to be based on the three Indicators 1 (time), 2 (complexity) and 3 (robustness).*

[0] Left invertibility deals with the question of recovering the full state of a system ("observation") together with some of its inputs ("unknown input observers"), and also refers to algebraic structural conditions.

[0] Note that hybrid dynamical systems (HDS) constitute an important field of investigation since, in this case, the discrete state can be considered as an unknown input.

3.3. Model-free control

Industry is keen on simple and powerful controllers: the tuning simplicity of the classical PID controller explains its omnipresence in industrial control systems, although its performances drop when working conditions change. The last challenge we consider is to define control techniques which, instead of using sophisticated models (the development of which may be expensive), use the information contained in the output signal and its estimated derivatives, which can be regarded as “signal-based” controllers. *Such design should take into account the Indicators 1 (time), 2 (complexity) and 3 (robustness).*

3.4. Applications

Keeping in mind that we will remain focused at developing and applying fundamental methods for non-asymptotic estimation, we intend to deal with 4 main domains of application (see the lower part of Figure 1). The Lille context offers interesting opportunities in WSAN (wireless sensor and actuator networks and, more particularly, networked robots) at Inria, as well as nano/macro machining at ENSAM. A power electronics platform will be developed in ENSEA Cergy. Last, in contact with companies, several grants, patents and collaborations are expected from the applications of $i-$PID. Each of these four application domains was presented in the *Non-A* proposal:

- Networked robots, WSAN [Lille]
- Nano/macro machining [Lille]
- Multicell chopper [Lille and Cergy]
- i-PID for industry

In the present period, we choose to give a particular focus to the first item (Networked robots), which already received some development. It can be considered as the objective 4.

POEMS Project-Team

3. Research Program

3.1. General description

Our activity relies on the existence of boundary value problems established by physicists to model the propagation of waves in various situations. The basic ingredient is a partial differential equation of the hyperbolic type, whose prototype is the wave equation (or the Helmholtz equation if time-periodic solutions are considered). Nowadays, the numerical techniques for solving the basic academic problems are well mastered. However, the solution of complex wave propagation problems close to real applications still raises (essentially open) problems which constitute a real challenge for applied mathematicians. In particular, several difficulties arise when extending the results and the methods from the scalar wave equation to vectorial problems modeling wave propagation in electromagnetism or elastodynamics.

A large part of research in mathematics, when applied to wave propagation problems, is oriented towards the following goals:

- The design of new numerical methods, increasingly accurate and efficient.
- The development of artificial transparent boundary conditions for handling unbounded propagation domains.
- The treatment of more and more complex configurations (non local models, non linear models, coupled systems, periodic media).
- The study of specific phenomena such as guided waves and resonances, which raise mathematical questions of spectral theory.
- The development of approximate models via asymptotic analysis with multiple scales (thin layers, boundary layers effects, small heterogeneities, homogenization, ...).
- The development and the analysis of algorithms for inverse problems (in particular for inverse scattering problems) and imaging techniques, using data from wave phenomena.

3.2. New schemes for time-domain simulations

Problems of wave propagation naturally arise as problems of evolution and it is necessary to have efficient methods for the calculation of their solution, directly in the time domain. The development and analysis of such methods has been in the past an important part of POEMS activity. Nowadays, there exists a large variety of higher order numerical methods that allow us to solve with good accuracy and in short computational time most classical wave propagation problems. However, when on wishes to deal with real life applications, one has to tackle problems which are complex in many ways: they involve multi-physics, non standard (possibly nonlinear) constitutive laws, highly heterogeneous media with high contrasts of coefficients, complex geometries... In many cases, such problems escape to the direct application of the above mentioned methods and ad hoc dedicated methods have to be designed. Such methods are most often of hybrid nature, which includes domain decomposition methods and subgridding, mixing of integral equations and PDEs, and artificial boundary conditions. In time domain, a particularly challenging issue is the time stability, in particular concerning the coupling of algorithms. To cope with this major difficulty, a key issue (and a kind of graal for numerical analysts) is the development of energy preserving methods which is one of the specificity of the research developed at POEMS in this field.

3.3. Integral equations

Our activity in this field aims at developing accurate and fast methods for 3D problems.

On one hand, we developed a systematic approach to the analytical evaluation of singular integrals, which arise in the computation of the matrices of integral equations when two elements of the mesh are either touching each other or geometrically close.

On the other hand, POEMS is developing Fast Boundary Element Methods for 3D acoustics or elastodynamics, with applications to soil-structure interaction, seismology or seismic imaging.

Finally, a posteriori error analysis methodologies and adaptivity for boundary integral equation formulations of acoustic, electromagnetic and elastic wave propagation is investigated in the framework of the ANR project RAFFINE.

3.4. Domain decomposition methods

This is a come back to a topic in which POEMS contributed in the 1990's. It is motivated by our collaborations with the CEA-CESTA and the CEA-LIST, for the solution of large problems in time-harmonic electromagnetism and elastodynamics.

We combine in an original manner classical ideas of Domain Decomposition Methods with the specific formulations that we use for wave problems in unbounded domains, taking benefit of the available analytical representations of the solution (integral representation, modal expansion etc...).

One ANR project (NonLocalDD) supports this research.

3.5. Wave propagation in complex media

Our objective is first to develop efficient numerical approaches for the propagation of waves in heterogeneous media, taking into account their complex microstructure.

We aim on one hand to improve homogenized modeling of periodic media, by deriving enriched boundary conditions (or transmission conditions if the periodic structure is embedded in a homogeneous matrix) which take into account the boundary layer phenomena. On the other hand, we like to develop multi-scale numerical methods when the assumption of periodicity on the spatial distribution of the heterogeneities is relaxed, or even completely lost. The general idea consists in a coupling between a macroscopic solver, based on a coarse mesh, with some microscopic representation of the field. This latter can be obtained by a numerical microscopic solver or by an analytical asymptotic expansion. This leads to two very different approaches which may be relevant for very different applications.

Extraordinary phenomena regarding the propagation of electromagnetic or acoustic waves appear in materials which have non classical properties: materials with a complex periodic microstructure that behave as materials with negative physical parameters, metals with a negative dielectric permittivity at optical frequencies, magnetized plasmas endowed with a strongly anisotropic and sign-indefinite permittivity tensor. These non classical materials raise original questions from theoretical and numerical points of view.

The objective is to study the well-posedness in this unusual context where physical parameters are sign-changing. New functional frameworks must be introduced, due, for instance, to hypersingularities of the electromagnetic field which appear at corners of metamaterials. This has of course numerical counterparts. In particular, classical Perfectly Matched Layers are unstable in these dispersive media, and new approaches must be developed.

Two ANR projects (METAMATH and CHROME) are related to this activity.

3.6. Spectral theory and modal approaches

The study of waveguides is a longstanding and major topic of the team. Concerning the selfadjoint spectral theory for open waveguides, we turned recently to the very important case of periodic media. One objective is to design periodic structures with localized perturbations to create gaps in the spectrum, containing isolating eigenvalues.

Then, we would like to go further in proving the absence of localized modes in non uniform open waveguides. An original approach has been successfully applied to the scalar problem of a waveguides junctions or bent waveguides. The challenge now is to extend these ideas to vectorial problems (for applications to electromagnetism or elastodynamics) and to junctions of periodic waveguides.

Besides, we will continue our activity on modal methods for closed waveguides. In particular, we aim at extending the enriched modal method to take into account curvature and rough boundaries.

Finally, we are developing asymptotic models for networks of thin waveguides which arise in several applications (electric networks, simulation of lung, nanophotonics...).

The study of waveguides is a longstanding and major topic of the team.

On this topic, a workshop entitled « New trends in theoretical and numerical analysis of waveguides » was co-organized by Anne-Sophie Bonnet-Ben Dhia (and Philippe Briet and Eric Soccrosi from CPT, Marseille and Michel Cristofol from I2M, Marseille) at IGESA (Porquerolles) from May 16th to 19th. This workshop is part of series of workshops organised from 2011 (in 2011 at Irmar, Rennes, in 2012 at Marseille, in 2013 at POems, Palaiseau, in 2015 at Napoli). The aim of these workshops is to bring together researchers from Mathematics, mathematical physics, theoretical physics and numerical analysis in order to encourage and stimulate the interactions between the different communities on problems associated to waveguides.

3.7. Inverse problems

Building on the strong expertise of POEMS in the mathematical modeling of waves, most of our contributions aim at improving inverse scattering methodologies.

We acquired some expertise on the so called Linear Sampling Method, from both the theoretical and the practical points of view. Besides, we are working on topological derivative methods, which exploit small-defect asymptotics of misfit functionals and can thus be viewed as an alternative sampling approach, which can take benefit of our expertise on asymptotic methods.

An originality of our activity is to consider inverse scattering in waveguides (the inverse scattering community generally considers only free-space configurations). This is motivated at the same time by specific issues concerning the ill-posedness of the identification process and by applications to non-destructive techniques, for waveguide configurations (cables, pipes, plates etc...).

Lastly, we continue our work on the so-called exterior approach for solving inverse obstacle problems, which associates quasi-reversibility and level set methods. The objective is now to extend it to evolution problems.

QUANTIC Project-Team

3. Research Program

3.1. Towards microwave quantum networks

The classical states of microwave radiation, are the so-called coherent states. They can be prepared by a commercial microwave generator (frequency 1GHz $< f <$ 20GHz) followed by thermalization to $k_BT \ll hf$ using a chain of attenuators anchored at various stages of a dilution refrigerator.

Owing to the strength of its coupling to superconducting circuits [53] or Rydberg atoms [70], microwave radiation can also be prepared in many possible non-classical states. Using a sequence of quanta exchanges between superconducting qubits and a microwave cavity, the direct preparation of an arbitrary superposition of Fock states has been demonstrated in 2009 [72] with about 90% fidelity up to 5 photons. Recently, the physicists at Yale university in collaboration with the theorists of QUANTIC team, demonstrated a superposition of classical states, or Schrödinger cat, with 100 photons on average, using the dispersive coupling to a transmon qubit [121].

An important class of states for quantum information processing with continuous variables is that of the Gaussian squeezed states [122]. These states can be seen as a coherent state for which the fluctuations on a quadrature are less than the zero point fluctuations. Of course, owing to Heisenberg uncertainty principle, this comes at the expense of larger fluctuations on the conjugated quadrature. In the optical domain, Gaussian light has been demonstrated and used with single and multimodes decades ago [122]. In the microwave domain, single mode squeezing of thermal noise had been demonstrated already in 1988 [127] but vacuum noise squeezing was only demonstrated in 2008 [50]. Since then, several groups have been able to generate single- and two-mode squeezing of microwave radiation, including us [57], [124], [88], [92], [59]. The two-mode squeezed states are of particular interest for quantum information processing, because they are maximally entangled for a given average number of quanta. In particular, the circuit developed by QUANTIC's experimentalists is able to directly generate two-mode squeezed states on separate transmission lines, at arbitrarily different frequencies [59].

In the perspective of a quantum network using microwave radiation, one needs a way to store and preserve microwave fields in nodes. Arguably, creating a memory for quantum systems able to preserve indefinitely a quantum state is the next big challenge on the road towards quantum computing [54], yet unrealized in any system. In a first step, we focus on a quantum node able to preserve a quantum state for a finite time.

In the optical domain, current implementations of quantum memories [112] rely mainly on two physical effects: the light deceleration due to electromagnetically induced transparency and the transfer of photonic quantum states onto collective atomic coherences (optical or spin). In the microwave domain, several quantum memories have emerged in the last years using spin ensembles [125], [78], [107], mechanical resonators [96], [97] or superconducting circuits [126], [123], such as our device described in [60].

All these microwave implementations have pros and cons. However, only two of them, the mechanical oscillator of the Lehnert group [97] and our device [60] have demonstrated entanglement between the memory and a propagating microwave mode. Specifically, our device consists in a 3D storage microwave cavity whose coupling to a transmission line is performed using an active superconducting circuit: the Josephson ring modulator. In the frequency conversion regime, it acts as a tunable coupler whose rate is solely controlled by the amplitude of a pump signal. In the parametric down-conversion regime, it acts as an entanglement generator, similarly to the mechanical version of the Boulder group. However, the inherently small coupling rate between the transmission line and the mechanical resonator in [97] makes our device [60] a much stronger candidate for a quantum node. Apart from this crucial possibility to generate entanglement, our device is similar to the implementation of Santa Barbara [126]. Both have demonstrated fast tuning (up to 30 MHz for Santa Barbara) with high catching efficiency and storage time of 4 μs. However we believe that two specificities make our route more promising. In their case it is a flux knob which allows tuning of the transparency of a 2D microwave cavity. The core of the device we propose is a 3D storage microwave, an architecture where there is plenty of room to improve the storage time and exceed this figure by orders of magnitude, even without quantum error correction [101]. Moreover the cavity transparency is controlled solely by the amplitude of a microwave tone, free of the complications of hysteresis inherent to fast flux tuning in a superconducting environment.

The quantum information protocols one can envision using the quantum node developed by QUANTIC's experimentalists gets a useful inspiration from what has been realized in the optical domain in the last 20 years. One of the most interesting protocols we would like to implement is the teleportation of a quantum state from the memory into a transmission line or another memory. In optics, this was performed already in 1998 for a coherent state [61], and more recently for a Schrödinger-cat-like state [79]. We could readily reproduce these experiments in the microwave regime. The deterministic teleportation of a superconducting quantum bit was realized only in 2013 [116] but no experiments have shown teleportation of a continuous variable state in the microwave domain up to now. Furthermore, none of the protocols needed for quantum information processing (entanglement distillation and dilution for instance) have ever been realized in the microwave domain with Gaussian states [122]. It is thus of great interest to investigate where the tools specific to superconducting circuits will allow us to go beyond what can be done in the optical domain. In particular, the microwave quantum limited amplifiers [104] developed by QUANTIC's experimentalists lead to unmatched heterodyne measurement efficiencies. Finally using a qubit as a Fock number resolved photocounter unleashes many scenarios in the preparation and manipulation by measurement of an entangled state [93].

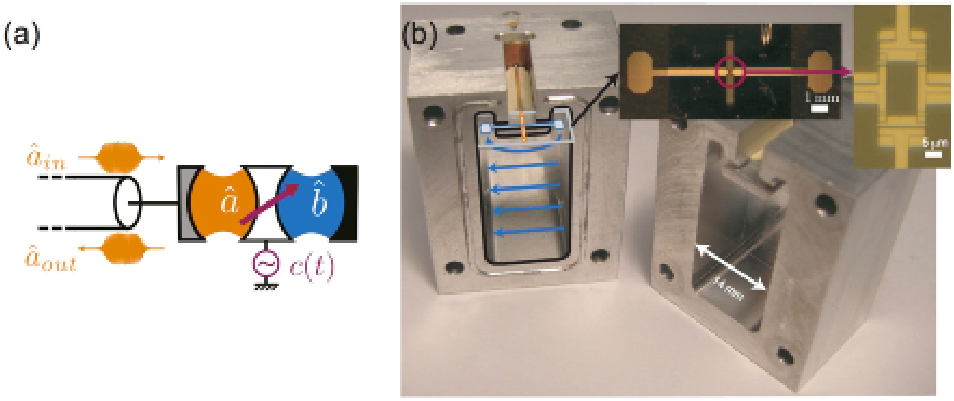


Figure 1. (a) Scheme of the quantum memory. A three-wave mixer is used as a controllable switch between a read/write cavity a and a long storage time cavity b *via the application of a control field c. (b) Picture of the first device. A 2D microstrip resonator on a Sapphire chip is dynamically coupled to a 3D aluminum cavity mode through antennas attached to a ring of 4 Josephson junctions.*

3.2. Hardware-efficient quantum information processing

In this scientific program, we will explore various theoretical and experimental issues concerning protection and manipulation of quantum information. Indeed, the next, critical stage in the development of Quantum Information Processing (QIP) is most certainly the active quantum error correction (QEC). Through this stage one designs, possibly using many physical qubits, an encoded logical qubit which is protected against major decoherence channels and hence admits a significantly longer effective coherence time than a physical qubit.

Reliable (fault-tolerant) computation with protected logical qubits usually comes at the expense of a significant overhead in the hardware (up to thousands of physical qubits per logical qubit). Each of the involved physical qubits still needs to satisfy the best achievable properties (coherence times, coupling strengths and tunability). More remarkably, one needs to avoid undesired interactions between various subsystems. This is going to be a major difficulty for qubits on a single chip.

The usual approach for the realization of QEC is to use many qubits to obtain a larger Hilbert space of the qubit register [111], [115]. By redundantly encoding quantum information in this Hilbert space of larger dimension one make the QEC tractable: different error channels lead to distinguishable error syndromes. There are two major drawbacks in using multi-qubit registers. The first, fundamental, drawback is that with each added physical qubit, several new decoherence channels are added. Because of the exponential increase of the Hilbert's space dimension versus the linear increase in the number of decay channels, using enough qubits, one is able to eventually protect quantum information against decoherence. However, multiplying the number of possible errors, this requires measuring more error syndromes. Note furthermore that, in general, some of these new decoherence channels can lead to correlated action on many qubits and this needs to be taken into account with extra care: in particular, such kind of non-local error channels are problematic for surface codes. The second, more practical, drawback is that it is still extremely challenging to build a register of more than on the order of 10 qubits where each of the qubits is required to satisfy near the best achieved properties: these properties include the coherence time, the coupling strengths and the tunability. Indeed, building such a register is not merely only a fabrication task but rather, one requirers to look for architectures such that, each individual qubit can be addressed and controlled independently from the others. One is also required to make sure that all the noise channels are well-controlled and uncorrelated for the QEC to be effective.

We have recently introduced a new paradigm for encoding and protecting quantum information in a quantum harmonic oscillator (e.g. a high-Q mode of a 3D superconducting cavity) instead of a multi-qubit register [81]. The infinite dimensional Hilbert space of such a system can be used to redundantly encode quantum information. The power of this idea lies in the fact that the dominant decoherence channel in a cavity is photon damping, and no more decay channels are added if we increase the number of photons we insert in the cavity. Hence, only a single error syndrome needs to be measured to identify if an error has occurred or not. Indeed, we are convinced that most early proposals on continuous variable QIP [76], [68] could be revisited taking into account the design flexibilities of Quantum Superconducting Circuits (QSC) and the new coupling regimes that are provided by these systems. In particular, we have illustrated that coupling a qubit to the cavity mode in the strong dispersive regime provides an important controllability over the Hilbert space of the cavity mode [80]. Through a recent experimental work [121], we benefit from this controllability to prepare superpositions of quasi-orthogonal coherent states, also known as Schrödinger cat states.

In this Scheme, the logical qubit is encoded in a four-component Schrödinger cat state. Continuous quantum non-demolition (QND) monitoring of a single physical observable, consisting of photon number parity, enables then the tractability of single photon jumps. We obtain therefore a first-order quantum error correcting code using only a single high-Q cavity mode (for the storage of quantum information), a single qubit (providing the non-linearity needed for controllability) and a single low-Q cavity mode (for reading out the error syndrome). An earlier experiment on such QND photon-number parity measurements [117] has recently led to a first experimental realization of a full quantum error correcting code improving the coherence time of quantum information [6]. As shown in Figure 2 , this leads to a significant hardware economy for realization of a protected logical qubit. Our goal here is to push these ideas towards a reliable and hardware-efficient paradigm for universal quantum computation.

3.3. Reservoir (dissipation) engineering and autonomous stabilization of quantum systems

Being at the heart of any QEC protocol, the concept of feedback is central for the protection of the quantum information enabling many-qubit quantum computation or long-distance quantum communication. However, such a closed-loop control which requires a real-time and continuous measurement of the quantum system has been for long considered as counter-intuitive or even impossible. This thought was mainly caused by

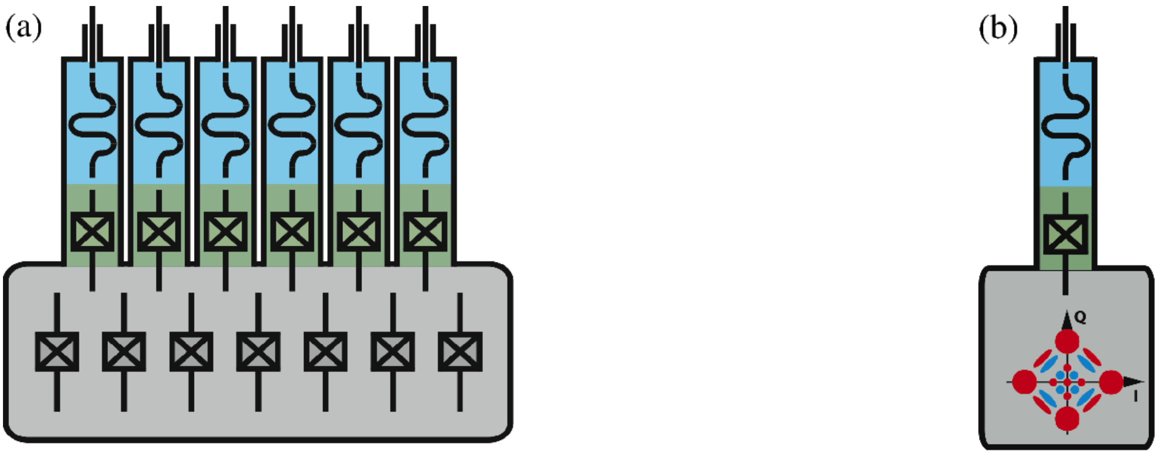


Figure 2. (a) A protected logical qubit consisting of a register of many qubits: here, we see a possible architecture for the Steane code [115] consisting of 7 qubits requiring the measurement of 6 error syndromes. In this sketch, 7 transmon qubits in a high-Q resonator and the measurement of the 6 error syndromes is ensured through 6 additional ancillary qubits with the possibility of individual readout of the ancillary qubits via independent low-Q resonators. (b) Minimal architecture for a protected logical qubit, adapted to circuit quantum electrodynamics experiments. Quantum information is encoded in a Schrödinger cat state of a single high-Q resonator mode and a single error syndrome is measured, using a single ancillary transmon qubit and the associated readout low-Q resonator.

properties of quantum measurements: any measurement implies an instantaneous strong perturbation to the system's state. The concept of *quantum non-demolotion* (QND) measurement has played a crucial role in understanding and resolving this difficulty [44]. In the context of cavity quantum electro-dynamics (cavity QED) with Rydberg atoms [70], a first experiment on continuous QND measurements of the number of microwave photons was performed by the group at Laboratoire Kastler-Brossel (ENS) [69]. Later on, this ability of performing continuous measurements allowed the same group to realize the first continuous quantum feedback protocol stabilizing highly non-classical states of the microwave field in the cavity, the so-called photon number states [8] (this ground-breaking work was mentioned in the Nobel prize attributed to Serge Haroche). The QUANTIC team contributed to the theoretical work behind this experiment [56], [35], [114], [37]. These contributions include the development and optimization of the quantum filters taking into account the quantum measurement back-action and various measurement noises and uncertainties, the development of a feedback law based on control Lyapunov techniques, and the compensation of the feedback delay.

In the context of circuit quantum electrodynamics (circuit QED) [55], recent advances in quantum-limited amplifiers [104], [119] have opened doors to high-fidelity non-demolition measurements and real-time feedback for superconducting qubits [71]. This ability to perform high-fidelity non-demolition measurements of a quantum signal has very recently led to quantum feedback experiments with quantum superconducting circuits [119], [103], [46]. Here again, the QUANTIC team has participated to one of the first experiments in the field where the control objective is to track a dynamical trajectory of a single qubit rather than stabilizing a stationary state. Such quantum trajectory tracking could be further explored to achieve metrological goals such as the stabilization of the amplitude of a microwave drive [89].

While all this progress has led to a strong optimism about the possibility to perform active protection of quantum information against decoherence, the rather short dynamical time scales of these systems limit, to a great amount, the complexity of the feedback strategies that could be employed. Indeed, in such measurement-based feedback protocols, the time-consuming data acquisition and post-treatment of the output signal leads to an important latency in the feedback procedure.

The reservoir (dissipation) engineering [100] and the closely related coherent feedback [86] are considered as alternative approaches circumventing the necessity of a real-time data acquisition, signal processing and feedback calculations. In the context of quantum information, the decoherence, caused by the coupling of a system to uncontrolled external degrees of freedom, is generally considered as the main obstacle to synthesize quantum states and to observe quantum effects. Paradoxically, it is possible to intentionally engineer a particular coupling to a reservoir in the aim of maintaining the coherence of some particular quantum states. In a general viewpoint, these approaches could be understood in the following manner: by coupling the quantum system to be stabilized to a strongly dissipative ancillary quantum system, one evacuates the entropy of the main system through the dissipation of the ancillary one. By building the feedback loop into the Hamiltonian, this type of autonomous feedback obviates the need for a complicated external control loop to correct errors. On the experimental side, such autonomous feedback techniques have been used for qubit reset [67], single-qubit state stabilization [91], and the creation [39] and stabilization [77], [85][9] of states of multipartite quantum systems.

Such reservoir engineering techniques could be widely revisited exploring the flexibility in the Hamiltonian design for QSC. We have recently developed theoretical proposals leading to extremely efficient, and simple to implement, stabilization schemes for systems consisting of a single, two or three qubits [67], [83], [51]. The experimental results based on these protocols have illustrated the efficiency of the approach [67][9]. Through these experiments, we exploit the strong dispersive interaction [109] between superconducting qubits and a single low-Q cavity mode playing the role of a dissipative reservoir. Applying some continuous-wave (cw) microwave drives with well-chosen fixed frequencies, amplitudes, and phases, we engineer an effective interaction Hamiltonian which evacuates entropy from the qubits when an eventual perturbation occurs: by driving the qubits and cavity with continuous-wave drives, we induce an autonomous feedback loop which corrects the state of the qubits every time it decays out of the desired target state. The schemes are robust against small variations of the control parameters (drives amplitudes and phase) and require only some basic calibration. Finally, by avoiding resonant interactions between the qubits and the low-Q cavity mode, the qubits remain protected against the Purcell effect, which would reduce the coherence times. We have also investigated both theoretically and experimentally the autonomous stabilization of non-classical states (such as Schrodinger cat states and Fock states) of microwave field confined in a high-Q cavity mode [90], [106], [73][5].

3.4. System theory for quantum information processing

In parallel and in strong interactions with the above experimental goals, we develop systematic mathematical methods for dynamical analysis, control and estimation of composite and open quantum systems. These systems are built with several quantum subsystems whose irreversible dynamics results from measurements and/or decoherence. A special attention is given to spin/spring systems made with qubits and harmonic oscillators. These developments are done in the spirit of our recent contributions [105], [35], [113], [108], [114], [37][7] resulting from collaborations with the cavity quantum electrodynamics group of Laboratoire Kastler Brossel.

3.4.1. Stabilization by measurement-based feedback

The protection of quantum information via efficient QEC is a combination of (i) tailored dynamics of a quantum system in order to protect an informational qubit from certain decoherence channels, and (ii) controlled reaction to measurements that efficiently detect and correct the dominating disturbances that are not rejected by the tailored quantum dynamics.

In such feedback scheme, the system and its measurement are quantum objects whereas the controller and the control input are classical. The stabilizing control law is based on the past values of the measurement outcomes. During our work on the LKB photon box, we have developed, for single input systems subject to quantum non-demolition measurement, a systematic stabilization method [37]: it is based on a discrete-time formulation of the dynamics, on the construction of a strict control Lyapunov function and on an explicit compensation of the feedback-loop delay. Keeping the QND measurement assumptions, extensions of such stabilization schemes will be investigated in the following directions: finite set of values for the control input with application to the convergence analysis of the atomic feedback scheme experimentally tested in [128]; multi-input case where the construction by inversion of a Metzler matrix of the strict Lyapunov function is not straightforward; continuous-time systems governed by diffusive master equations; stabilization towards a set of density operators included in a target subspace; adaptive measurement by feedback to accelerate the convergence towards a stationary state as experimentally tested in [98]. Without the QND measurement assumptions, we will also address the stabilization of non-stationary states and trajectory tracking, with applications to systems similar to those considered in [71], [46].

3.4.2. Filtering, quantum state and parameter estimations

The performance of every feedback controller crucially depends on its online estimation of the current situation. This becomes even more important for quantum systems, where full state measurements are physically impossible. Therefore the ultimate performance of feedback correction depends on fast, efficient and optimally accurate state and parameter estimations.

A quantum filter takes into account imperfection and decoherence and provides the quantum state at time $t \geq 0$ from an initial value at $t = 0$ and the measurement outcomes between 0 and t. Quantum filtering goes back to the work of Belavkin [40] and is related to quantum trajectories [48], [52]. A modern and mathematical exposure of the diffusive models is given in [38]. In [129] a first convergence analysis of diffusive filters is proposed. Nevertheless the convergence characterization and estimation of convergence rate remain open and difficult problems. For discrete time filters, a general stability result based on fidelity is proven in [105], [113]. This stability result is extended to a large class of continuous-time filters in [36]. Further efforts are required to characterize asymptotic and exponential stability. Estimations of convergence rates are available only for quantum non-demolition measurements [41]. Parameter estimations based on measurement data of quantum trajectories can be formulated within such quantum filtering framework [62], [94].

We will continue to investigate stability and convergence of quantum filtering. We will also exploit our fidelity-based stability result to justify maximum likelihood estimation and to propose, for open quantum system, parameter estimation algorithms inspired of existing estimation algorithms for classical systems. We will also investigate a more specific quantum approach: it is noticed in [45] that post-selection statistics and "past quantum" state analysis [63] enhance sensitivity to parameters and could be interesting towards increasing the precision of an estimation.

3.4.3. Stabilization by interconnections

In such stabilization schemes, the controller is also a quantum object: it is coupled to the system of interest and is subject to decoherence and thus admits an irreversible evolution. These stabilization schemes are closely related to reservoir engineering and coherent feedback [100], [86]. The closed-loop system is then a composite system built with the original system and its controller. In fact, and given our particular recent expertise in this domain [7], [9] [67], this subsection is dedicated to further developing such stabilization techniques, both experimentally and theoretically.

The main analysis issues are to prove the closed-loop convergence and to estimate the convergence rates. Since these systems are governed by Lindblad differential equations (continuous-time case) or Kraus maps (discrete-time case), their stability is automatically guaranteed: such dynamics are contractions for a large set of metrics (see [99]). Convergence and asymptotic stability is less well understood. In particular most of the convergence results consider the case where the target steady-state is a density operator of maximum rank (see, e.g., [34][chapter 4, section 6]). When the goal steady-state is not full rank very few convergence results are available.

We will focus on this geometric situation where the goal steady-state is on the boundary of the cone of positive Hermitian operators of finite trace. A specific attention will be given to adapt standard tools (Lyapunov function, passivity, contraction and Lasalle's invariance principle) for infinite dimensional systems to spin/spring structures inspired of [7], [9] [67], [90] and their associated Fokker-Planck equations for the Wigner functions.

We will also explore the Heisenberg point of view in connection with recent results of the Inria project-team MAXPLUS (algorithms and applications of algebras of max-plus type) relative to Perron-Frobenius theory [66], [65]. We will start with [110] and [102] where, based on a theorem due to Birkhoff [42], dual Lindblad equations and dual Kraus maps governing the Heisenberg evolution of any operator are shown to be contractions on the cone of Hermitian operators equipped with Hilbert's projective metric. As the Heisenberg picture is characterized by convergence of all operators to a multiple of the identity, it might provide a mean to circumvent the rank issues. We hope that such contraction tools will be especially well adapted to analyzing quantum systems composed of multiple components, motivated by the facts that the same geometry describes the contraction of classical systems undergoing synchronizing interactions [118] and by our recent generalized extension of the latter synchronizing interactions to quantum systems [87].

Besides these analysis tasks, the major challenge in stabilization by interconnections is to provide systematic methods for the design, from typical building blocks, of control systems that stabilize a specific quantum goal (state, set of states, operation) when coupled to the target system. While constructions exist for so-called linear quantum systems [95], this does not cover the states that are more interesting for quantum applications. Various strategies have been proposed that concatenate iterative control steps for open-loop steering [120], [84] with experimental limitations. The characterization of Kraus maps to stabilize any types of states has also been established [43], but without considering experimental implementations. A viable stabilization by interaction has to combine the capabilities of these various approaches, and this is a missing piece that we want to address.

3.4.3.1. Perturbation methods

With this subsection we turn towards more fundamental developments that are necessary in order to address the complexity of quantum networks with efficient reduction techniques. This should yield both efficient mathematical methods, as well as insights towards unravelling dominant physical phenomena/mechanisms in multipartite quantum dynamical systems.

In the Schrödinger point of view, the dynamics of open quantum systems are governed by master equations, either deterministic or stochastic [70], [64]. Dynamical models of composite systems are based on tensor products of Hilbert spaces and operators attached to the constitutive subsystems. Generally, a hierarchy of different timescales is present. Perturbation techniques can be very useful to construct reliable models adapted to the timescale of interest.

To eliminate high frequency oscillations possibly induced by quasi-resonant classical drives, averaging techniques are used (rotating wave approximation). These techniques are well established for closed systems without any dissipation nor irreversible effect due to measurement or decoherence. We will consider in a first step the adaptation of these averaging techniques to deterministic Lindblad master equations governing the quantum state, i.e. the system density operator. Emphasis will be put on first order and higher order corrections based on non-commutative computations with the different operators appearing in the Lindblad equations. Higher order terms could be of some interest for the protected logical qubit of figure 2 b. In future steps, we intend to explore the possibility to explicitly exploit averaging or singular perturbation properties in the design of coherent quantum feedback systems; this should be an open-systems counterpart of works like [82].

To eliminate subsystems subject to fast convergence induced by decoherence, singular perturbation techniques can be used. They provide reduced models of smaller dimension via the adiabatic elimination of the rapidly converging subsystems. The derivation of the slow dynamics is far from being obvious (see, e.g., the computations of page 142 in [47] for the adiabatic elimination of low-Q cavity). Contrarily to the classical composite systems where we have to eliminate one component in a Cartesian product, we here have to eliminate one component in a tensor product. We will adapt geometric singular perturbations [58] and invariant manifold techniques [49] to such tensor product computations to derive reduced slow approximations of any order. Such adaptations will be very useful in the context of quantum Zeno dynamics to obtain approximations of the slow dynamics on the decoherence-free subspace corresponding to the slow attractive manifold.

Perturbation methods are also precious to analyze convergence rates. Deriving the spectrum attached to the Lindblad differential equation is not obvious. We will focus on the situation where the decoherence terms of the form $L\rho L^\dagger - (L^\dagger L\rho + \rho L^\dagger L)/2$ are small compared to the conservative terms $-i[H/\hbar, \rho]$. The difficulty to overcome here is the degeneracy of the unperturbed spectrum attached to the conservative evolution $\frac{d}{dt}\rho = -i[H/\hbar, \rho]$. The degree of degeneracy of the zero eigenvalue always exceeds the dimension of the Hilbert space. Adaptations of usual perturbation techniques [74] will be investigated. They will provide estimates of convergence rates for slightly open quantum systems. We expect that such estimates will help to understand the dependence on the experimental parameters of the convergence rates observed in [67][9] [83].

As particular outcomes for the other subsections, we expect that these developments towards simpler dominant dynamics will guide the search for optimal control strategies, both in open-loop microwave networks and in autonomous stabilization schemes such as reservoir engineering. It will further help to efficiently compute explicit convergence rates and quantitative performances for all the intended experiments.

RAPSODI Team

3. Research Program

3.1. Design and analysis of structure preserving schemes

3.1.1. Numerical analysis of nonlinear numerical methods

Up to now, the numerical methods dedicated to degenerate parabolic problems that the mathematicians are able to analyze almost all rely on the use of mathematical transformations (like e.g. the Kirchhoff's transform). It forbids the extension of the analysis to complex realistic models. The methods used in the industrial codes for solving such complex problems rely on the use of what we call NNM, i.e., on methods that preserve all the nonlinearities of the problem without reducing them thanks to artificial mathematical transforms. Our aim is to take advantage on the recent breakthrough proposed by C. Cancès & C. Guichard [16], [30] to develop efficient new numerical methods with a full numerical analysis (stability, convergence, error estimates, robustness w.r.t. physical parameters, ...).

3.1.2. Design and analysis of asymptotic preserving schemes

There has been an extensive effort in the recent years to develop numerical methods for diffusion equations that are robust with respect to heterogeneities, anisotropy, and the mesh (see for instance [58] for an extensive discussion on such methods). On the other hand, the understanding of the role of nonlinear stability properties in the asymptotic behaviors of dissipative systems increased significantly in the last decades (see for instance [51], [72]).

Recently, C. Chainais-Hillairet and co-authors [3], [8] and [19] developed a strategy based on the control of the numerical counterpart of the physical entropy to develop and analyze AP numerical methods. In particular, these methods show great promises for capturing accurately the behavior of the solutions to dissipative problems when some physical parameter is small with respect to the discretization characteristic parameters, or in the long-time asymptotic. Since it requires the use of nonlinear test functions in the analysis, strong restrictions on the physics (isotropic problems) and on the mesh (Cartesian grids, Voronoï boxes...) are required in [3], [8] and [19]. The schemes proposed in [16], [30] allow to handle nonlinear test functions in the analysis without restrictions on the mesh and on the anisotropy of the problem. Combining the nonlinear schemes *à la* [16] with the methodology of [3], [8], [19] would provide schemes that are robust both with respect to the meshes and to the parameters. Therefore, they would be also robust under adaptive mesh refinement.

3.1.3. Design and stability analysis of numerical methods for mixture problems

We aim at extending the range of the `NS2DDV-M` software by introducing new physical models, like for instance the Kazhikov and Smagulov model [68]. This will require a theoretical study for proving the existence of weak solutions to this model. Then, we will need to design numerical schemes to approximate these models and study their stability. We will also study their convergence following the path proposed in [62], [69].

3.2. Optimizing the computational efficiency

3.2.1. High order nonlinear numerical methods

The numerical experiments carried out in [16] show that in case of very strong anisotropy, the convergence of the proposed NNM becomes too slow (less than first order). Indeed, the method appears to strongly overestimate the dissipation. In order to make the method more competitive, it is necessary to estimate the dissipation in a more accurate way. Preliminary numerical results show that second order accuracy in space can be achieved in this way. One also aims to obtain (at least) second order accuracy in time without jeopardizing the stability. For many problems, this can be done by using so-called two-step backward differentiation formulas (BDF2) [59].

Concerning the inhomogeneous fluid models, we aim to investigate new methods for the mass equation resolution. Indeed, we aim at increasing the accuracy while maintaining some positivity-like properties and the efficiency for a wide range of physical parameters. To this end, we will consider *residual distribution* (RD) schemes, that appear as an alternative to finite volume methods. RD schemes enjoy very compact stencils. Therefore, their extension from 2D to 3D yield reasonable difficulties. These methods appeared twenty years ago, but recent extensions to unsteady problems [73], [64], with high-order accuracy [40], [39], or for parabolic problems [37], [38] make them very competitive. Relying on these breakthroughs, we aim at designing new RD schemes for fluid mixture models with high-order accuracy while preserving the positivity of the solutions.

3.2.2. A posteriori error control

The question of the *a posteriori* error estimators will also have to be addressed in this optimization context. Since the pioneering papers of Babuska and Rheinboldt more than thirty years ago [44], *a posteriori* error estimators have been widely studied. We will take advantage of the huge corresponding bibliography database in order to optimize our numerical results.

For example, we would like to generalize the results we derived for the harmonic magnetodynamic case (e.g. [10] and [52]) to the temporal magnetodynamic one, for which space/time *a posteriori* error estimators have to be developed. A space/time refinement algorithm should consequently be proposed and tested on academic as well as industrial benchmarks.

We also want to develop *a posteriori* estimators for the variable density Navier-Stokes model or some of its variants. To do so, several difficulties have to be tackled: the problem is nonlinear, unsteady, and the numerical method [5], [6] we developed combines features from finite elements and finite volumes. Fortunately, we do not start from scratch. Some recent references are devoted to the unsteady Navier-Stokes model in the finite element context [47], [77]. In the finite volume context, recent references deal with unsteady convection-diffusion equations [76], [43], [57] and [50]. We want to adapt some of these results to the variable density Navier-Stokes system, and to be able to design an efficient space-time remeshing algorithm.

3.2.3. Efficient computation of pairwise interactions in large systems of particles

Many systems are modeled as a large number of punctual individuals (N) which interact pairwise which means $N(N-1)/2$ interactions. Such systems are ubiquitous, they are found in chemistry (Van der Waals interaction between atoms), in astrophysics (gravitational interactions between stars, galaxies or galaxy clusters), in biology (flocking behavior of birds, swarming of fishes) or in the description of crowd motions. Building on the special structure of convolution type of the interactions, the team develops computation methods based on the Non Uniform Fast Fourier Transform [61]. This reduces the $O(N^2)$ naïve computational cost of the interactions to $O(N \log N)$, allowing numerical simulations involving millions of individuals.

REALOPT Project-Team

3. Research Program

3.1. Introduction

Combinatorial optimization is the field of discrete optimization problems. In many applications, the most important decisions (control variables) are binary (on/off decisions) or integer (indivisible quantities). Extra variables can represent continuous adjustments or amounts. This results in models known as *mixed integer programs* (MIP), where the relationships between variables and input parameters are expressed as linear constraints and the goal is defined as a linear objective function. MIPs are notoriously difficult to solve: good quality estimations of the optimal value (bounds) are required to prune enumeration-based global-optimization algorithms whose complexity is exponential. In the standard approach to solving an MIP is so-called *branch-and-bound algorithm* : (i) one solves the linear programming (LP) relaxation using the simplex method; (ii) if the LP solution is not integer, one adds a disjunctive constraint on a factional component (rounding it up or down) that defines two sub-problems; (iii) one applies this procedure recursively, thus defining a binary enumeration tree that can be pruned by comparing the local LP bound to the best known integer solution. Commercial MIP solvers are essentially based on branch-and-bound (such IBM-CPLEX, FICO-Xpress-mp, or GUROBI). They have made tremendous progress over the last decade (with a speedup by a factor of 60). But extending their capabilities remains a continuous challenge; given the combinatorial explosion inherent to enumerative solution techniques, they remain quickly overwhelmed beyond a certain problem size or complexity.

Progress can be expected from the development of tighter formulations. Central to our field is the characterization of polyhedra defining or approximating the solution set and combinatorial algorithms to identify "efficiently" a minimum cost solution or separate an unfeasible point. With properly chosen formulations, exact optimization tools can be competitive with other methods (such as meta-heuristics) in constructing good approximate solutions within limited computational time, and of course has the important advantage of being able to provide a performance guarantee through the relaxation bounds. Decomposition techniques are implicitly leading to better problem formulation as well, while constraint propagation are tools from artificial intelligence to further improve formulation through intensive preprocessing. A new trend is robust optimization where recent progress have been made: the aim is to produce optimized solutions that remain of good quality even if the problem data has stochastic variations. In all cases, the study of specific models and challenging industrial applications is quite relevant because developments made into a specific context can become generic tools over time and see their way into commercial software.

Our project brings together researchers with expertise in mathematical programming (polyhedral approaches, Dantzig-Wolfe decomposition, mixed integer programing, robust and stochastic programming, and dynamic programming), graph theory (characterization of graph properties, combinatorial algorithms) and constraint programming in the aim of producing better quality formulations and developing new methods to exploit these formulations. These new results are then applied to find high quality solutions for practical combinatorial problems such as routing, network design, planning, scheduling, cutting and packing problems.

3.2. Polyhedral approaches for MIP

Adding valid inequalities to the polyhedral description of an MIP allows one to improve the resulting LP bound and hence to better prune the enumeration tree. In a cutting plane procedure, one attempt to identify valid inequalities that are violated by the LP solution of the current formulation and adds them to the formulation. This can be done at each node of the branch-and-bound tree giving rise to a so-called *branch-and-cut algorithm* [64]. The goal is to reduce the resolution of an integer program to that of a linear program by deriving a linear description of the convex hull of the feasible solutions. Polyhedral theory tells us that if X is a mixed integer program: $X = P \cap \mathbb{Z}^n \times \mathbb{R}^p$ where $P = \{x \in \mathbb{R}^{n+p} : Ax \leq b\}$ with matrix

$(A, b) \in \mathbb{Q}^{m\times(n+p+1)}$, then $conv(X)$ is a polyhedron that can be described in terms of linear constraints, i.e. it writes as $conv(X) = \{x \in \mathbb{R}^{n+p} : C\,x \leq d\}$ for some matrix $(C, d) \in \mathbb{Q}^{m'\times(n+p+1)}$ although the dimension m' is typically quite large. A fundamental result in this field is the equivalence of complexity between solving the combinatorial optimization problem $\min\{cx : x \in X\}$ and solving the *separation problem* over the associated polyhedron $conv(X)$: if $\widetilde{x} \notin conv(X)$, find a linear inequality $\pi\,x \geq \pi_0$ satisfied by all points in $conv(X)$ but violated by $\widetilde{x}$. Hence, for NP-hard problems, one can not hope to get a compact description of $conv(X)$ nor a polynomial time exact separation routine. Polyhedral studies focus on identifying some of the inequalities that are involved in the polyhedral description of $conv(X)$ and derive efficient *separation procedures* (cutting plane generation). Only a subset of the inequalities $C\,x \leq d$ can offer a good approximation, that combined with a branch-and-bound enumeration techniques permits to solve the problem. Using *cutting plane algorithm* at each node of the branch-and-bound tree, gives rise to the algorithm called *branch-and-cut*.

3.3. Decomposition and reformulation approaches

An hierarchical approach to tackle complex combinatorial problems consists in considering separately different substructures (subproblems). If one is able to implement relatively efficient optimization on the substructures, this can be exploited to reformulate the global problem as a selection of specific subproblem solutions that together form a global solution. If the subproblems correspond to subset of constraints in the MIP formulation, this leads to Dantzig-Wolfe decomposition [1], [4], [5], [3]. If it corresponds to isolating a subset of decision variables, this leads to Bender's decomposition. Both lead to extended formulations of the problem with either a huge number of variables or constraints. Dantzig-Wolfe approach requires specific algorithmic approaches to generate subproblem solutions and associated global decision variables dynamically in the course of the optimization. This procedure is known as *column generation*, while its combination with branch-and-bound enumeration is called *branch-and-price*. Alternatively, in Bender's approach, when dealing with exponentially many constraints in the reformulation, the *cutting plane procedures* that we defined in the previous section are well-suited tools. When optimization on a substructure is (relatively) easy, there often exists a tight reformulation of this substructure typically in an extended variable space. This gives rise powerful reformulation of the global problem, although it might be impractical given its size (typically pseudo-polynomial). It can be possible to project (part of) the extended formulation in a smaller dimensional space if not the original variable space to bring polyhedral insight (cuts derived through polyhedral studies can often be recovered through such projections).

3.4. Integration of Artificial Intelligence Techniques in Integer Programming

When one deals with combinatorial problems with a large number of integer variables, or tightly constrained problems, mixed integer programming (MIP) alone may not be able to find solutions in a reasonable amount of time. In this case, techniques from artificial intelligence can be used to improve these methods. In particular, we use primal heuristics and constraint programming.

Primal heuristics are useful to find feasible solutions in a small amount of time. We focus on heuristics that are either based on integer programming (rounding, diving, relaxation induced neighborhood search, feasibility pump), or that are used inside our exact methods (heuristics for separation or pricing subproblem, heuristic constraint propagation, ...).

Constraint Programming (CP) focuses on iteratively reducing the variable domains (sets of feasible values) by applying logical and problem-specific operators. The latter propagates on selected variables the restrictions that are implied by the other variable domains through the relations between variables that are defined by the constraints of the problem. Combined with enumeration, it gives rise to exact optimization algorithms. A CP approach is particularly effective for tightly constrained problems, feasibility problems and min-max problems Mixed Integer Programming (MIP), on the other hand, is known to be effective for loosely constrained problems and for problems with an objective function defined as the weighted sum of variables. Many problems belong to the intersection of these two classes. For such problems, it is reasonable to use algorithms that exploit complementary strengths of Constraint Programming and Mixed Integer Programming.

3.5. Robust Optimization

Decision makers are usually facing several sources of uncertainty, such as the variability in time or estimation errors. A simplistic way to handle these uncertainties is to overestimate the unknown parameters. However, this results in over-conservatism and a significant waste in resource consumption. A better approach is to account for the uncertainty directly into the decision aid model by considering mixed integer programs that involve uncertain parameters. Stochastic optimization account for the expected realization of random data and optimize an expected value representing the average situation. Robust optimization on the other hand entails protecting against the worst-case behavior of unknown data. There is an analogy to game theory where one considers an oblivious adversary choosing the realization that harms the solution the most. A full worst case protection against uncertainty is too conservative and induces very high over-cost. Instead, the realization of random data are bound to belong to a restricted feasibility set, the so-called uncertainty set. Stochastic and robust optimization rely on very large scale programs where probabilistic scenarios are enumerated. There is hope of a tractable solution for realistic size problems, provided one develops very efficient ad-hoc algorithms. The techniques for dynamically handling variables and constraints (column-and-row generation and Bender's projection tools) that are at the core of our team methodological work are specially well-suited to this context.

3.6. Polyhedral Combinatorics and Graph Theory

Many fundamental combinatorial optimization problems can be modeled as the search for a specific structure in a graph. For example, ensuring connectivity in a network amounts to building a *tree* that spans all the nodes. Inquiring about its resistance to failure amounts to searching for a minimum cardinality *cut* that partitions the graph. Selecting disjoint pairs of objects is represented by a so-called *matching*. Disjunctive choices can be modeled by edges in a so-called *conflict graph* where one searches for *stable sets* – a set of nodes that are not incident to one another. Polyhedral combinatorics is the study of combinatorial algorithms involving polyhedral considerations. Not only it leads to efficient algorithms, but also, conversely, efficient algorithms often imply polyhedral characterizations and related min-max relations. Developments of polyhedral properties of a fundamental problem will typically provide us with more interesting inequalities well suited for a branch-and-cut algorithm to more general problems. Furthermore, one can use the fundamental problems as new building bricks to decompose the more general problem at hand. For problem that let themselves easily be formulated in a graph setting, the graph theory and in particular graph decomposition theorem might help.

SELECT Project-Team

3. Research Program

3.1. General presentation

From applications we treat on a day-to-day basis, we have learned that some assumptions currently used in asymptotic theory for model selection are often irrelevant in practice. For instance, it is not realistic to assume that the target belongs to the family of models in competition. Moreover, in many situations, it is useful to make the size of the model depend on the sample size, which makes asymptotic analyses breakdown. An important aim of SELECT is to propose model selection criteria which take such practical constraints into account.

3.2. A nonasymptotic view of model selection

An important goal of SELECT is to build and analyze penalized log-likelihood model selection criteria that are efficient when the number of models in competition grows to infinity with the number of observations. Concentration inequalities are a key tool for this, and lead to data-driven penalty choice strategies. A major research direction for SELECT consists of deepening the analysis of data-driven penalties, both from the theoretical and practical points of view. There is no universal way of calibrating penalties, but there are several different general ideas that we aim to develop, including heuristics derived from Gaussian theory, special strategies for variable selection, and resampling methods.

3.3. Taking into account the modeling purpose in model selection

Choosing a model is not only difficult theoretically. From a practical point of view, it is important to design model selection criteria that accommodate situations in which the data probability distribution P is unknown, and which take the model user's purpose into account. Most standard model selection criteria assume that P belongs to one of a set of models, without considering the purpose of the model. By also considering the model user's purpose, we can avoid or overcome certain theoretical difficulties, and produce flexible model selection criteria with data-driven penalties. The latter is useful in supervised classification and hidden-structure models.

3.4. Bayesian model selection

The Bayesian approach to statistical problems is fundamentally probabilistic: a joint probability distribution is used to describe the relationships among all unknowns and the data. Inference is then based on the posterior distribution, i.e., the conditional probability distribution of the parameters given the observed data. Exploiting the internal consistency of the probability framework, the posterior distribution extracts relevant information in the data and provides a complete and coherent summary of post-data uncertainty. Using the posterior to solve specific inference and decision problems is then straightforward, at least in principle.

SEQUEL Project-Team

3. Research Program

3.1. In Short

SEQUEL is primarily grounded on two domains:

- the problem of decision under uncertainty,
- statistical analysis and statistical learning, which provide the general concepts and tools to solve this problem.

To help the reader who is unfamiliar with these questions, we briefly present key ideas below.

3.2. Decision-making Under Uncertainty

The phrase “Decision under uncertainty” refers to the problem of taking decisions when we do not have a full knowledge neither of the situation, nor of the consequences of the decisions, as well as when the consequences of decision are non deterministic.

We introduce two specific sub-domains, namely the Markov decision processes which models sequential decision problems, and bandit problems.

3.2.1. Reinforcement Learning

Sequential decision processes occupy the heart of the SEQUEL project; a detailed presentation of this problem may be found in Puterman’s book [65].

A Markov Decision Process (MDP) is defined as the tuple $(\mathcal{X}, \mathcal{A}, P, r)$ where $\mathcal{X}$ is the state space, $\mathcal{A}$ is the action space, P is the probabilistic transition kernel, and $r : \mathcal{X} \times \mathcal{A} \times \mathcal{X} \to \mathbb{R}$ is the reward function. For the sake of simplicity, we assume in this introduction that the state and action spaces are finite. If the current state (at time t) is $x \in \mathcal{X}$ and the chosen action is $a \in \mathcal{A}$, then the Markov assumption means that the transition probability to a new state $x' \in \mathcal{X}$ (at time $t+1$) only depends on (x, a). We write $p(x'|x, a)$ the corresponding transition probability. During a transition $(x, a) \to x'$, a reward $r(x, a, x')$ is incurred.

In the MDP $(\mathcal{X}, \mathcal{A}, P, r)$, each initial state x_0 and action sequence $a_0, a_1, ...$ gives rise to a sequence of states $x_1, x_2, ...$, satisfying $\mathbb{P}\left(x_{t+1} = x'|x_t = x, a_t = a\right) = p(x'|x, a)$, and rewards [0]$r_1, r_2, ...$ defined by $r_t = r(x_t, a_t, x_{t+1})$.

The history of the process up to time t is defined to be $H_t = (x_0, a_0, ..., x_{t-1}, a_{t-1}, x_t)$. A policy π is a sequence of functions $\pi_0, \pi_1, ...$, where π_t maps the space of possible histories at time t to the space of probability distributions over the space of actions $\mathcal{A}$. To follow a policy means that, in each time step, we assume that the process history up to time t is $x_0, a_0, ..., x_t$ and the probability of selecting an action a is equal to $\pi_t(x_0, a_0, ..., x_t)(a)$. A policy is called stationary (or Markovian) if π_t depends only on the last visited state. In other words, a policy $\pi = (\pi_0, \pi_1, ...)$ is called stationary if $\pi_t(x_0, a_0, ..., x_t) = \pi_0(x_t)$ holds for all $t \geq 0$. A policy is called deterministic if the probability distribution prescribed by the policy for any history is concentrated on a single action. Otherwise it is called a stochastic policy.

[0] Note that for simplicity, we considered the case of a deterministic reward function, but in many applications, the reward r_t itself is a random variable.

We move from an MD process to an MD problem by formulating the goal of the agent, that is what the sought policy π has to optimize? It is very often formulated as maximizing (or minimizing), in expectation, some functional of the sequence of future rewards. For example, an usual functional is the infinite-time horizon sum of discounted rewards. For a given (stationary) policy π, we define the value function $V^{\pi}(x)$ of that policy π at a state $x \in \mathcal{X}$ as the expected sum of discounted future rewards given that we state from the initial state x and follow the policy π:

$$V^{\pi}(x) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t | x_0 = x, \pi\right], \tag{66}$$

where $\mathbb{E}$ is the expectation operator and $\gamma \in (0,1)$ is the discount factor. This value function V^{π} gives an evaluation of the performance of a given policy π. Other functionals of the sequence of future rewards may be considered, such as the undiscounted reward (see the stochastic shortest path problems [64]) and average reward settings. Note also that, here, we considered the problem of maximizing a reward functional, but a formulation in terms of minimizing some cost or risk functional would be equivalent.

In order to maximize a given functional in a sequential framework, one usually applies Dynamic Programming (DP) [62], which introduces the optimal value function $V^*(x)$, defined as the optimal expected sum of rewards when the agent starts from a state x. We have $V^*(x) = \sup_{\pi} V^{\pi}(x)$. Now, let us give two definitions about policies:

- We say that a policy π is optimal, if it attains the optimal values $V^*(x)$ for any state $x \in \mathcal{X}$, *i.e.*, if $V^{\pi}(x) = V^*(x)$ for all $x \in \mathcal{X}$. Under mild conditions, deterministic stationary optimal policies exist [63]. Such an optimal policy is written π^*.
- We say that a (deterministic stationary) policy π is greedy with respect to (w.r.t.) some function V (defined on $\mathcal{X}$) if, for all $x \in \mathcal{X}$,

$$\pi(x) \in \arg\max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V(x')\right].$$

  where $\arg\max_{a \in \mathcal{A}} f(a)$ is the set of $a \in \mathcal{A}$ that maximizes $f(a)$. For any function V, such a greedy policy always exists because $\mathcal{A}$ is finite.

The goal of Reinforcement Learning (RL), as well as that of dynamic programming, is to design an optimal policy (or a good approximation of it).

The well-known Dynamic Programming equation (also called the Bellman equation) provides a relation between the optimal value function at a state x and the optimal value function at the successors states x' when choosing an optimal action: for all $x \in \mathcal{X}$,

$$V^*(x) = \max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V^*(x')\right]. \tag{67}$$

The benefit of introducing this concept of optimal value function relies on the property that, from the optimal value function V^*, it is easy to derive an optimal behavior by choosing the actions according to a policy greedy w.r.t. V^*. Indeed, we have the property that a policy greedy w.r.t. the optimal value function is an optimal policy:

$$\pi^*(x) \in \arg\max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V^*(x')\right]. \tag{68}$$

In short, we would like to mention that most of the reinforcement learning methods developed so far are built on one (or both) of the two following approaches ([68]):

- Bellman's dynamic programming approach, based on the introduction of the value function. It consists in learning a "good" approximation of the optimal value function, and then using it to derive a greedy policy w.r.t. this approximation. The hope (well justified in several cases) is that the performance V^π of the policy π greedy w.r.t. an approximation V of V^* will be close to optimality. This approximation issue of the optimal value function is one of the major challenges inherent to the reinforcement learning problem. **Approximate dynamic programming** addresses the problem of estimating performance bounds (*e.g.* the loss in performance $||V^* - V^\pi||$ resulting from using a policy π-greedy w.r.t. some approximation V- instead of an optimal policy) in terms of the approximation error $||V^* - V||$ of the optimal value function V^* by V. Approximation theory and Statistical Learning theory provide us with bounds in terms of the number of sample data used to represent the functions, and the capacity and approximation power of the considered function spaces.
- Pontryagin's maximum principle approach, based on sensitivity analysis of the performance measure w.r.t. some control parameters. This approach, also called **direct policy search** in the Reinforcement Learning community aims at directly finding a good feedback control law in a parameterized policy space without trying to approximate the value function. The method consists in estimating the so-called **policy gradient**, *i.e.* the sensitivity of the performance measure (the value function) w.r.t. some parameters of the current policy. The idea being that an optimal control problem is replaced by a parametric optimization problem in the space of parameterized policies. As such, deriving a policy gradient estimate would lead to performing a stochastic gradient method in order to search for a local optimal parametric policy.

Finally, many extensions of the Markov decision processes exist, among which the Partially Observable MDPs (POMDPs) is the case where the current state does not contain all the necessary information required to decide for sure of the best action.

3.2.2. Multi-arm Bandit Theory

Bandit problems illustrate the fundamental difficulty of decision making in the face of uncertainty: A decision maker must choose between what seems to be the best choice ("exploit"), or to test ("explore") some alternative, hoping to discover a choice that beats the current best choice.

The classical example of a bandit problem is deciding what treatment to give each patient in a clinical trial when the effectiveness of the treatments are initially unknown and the patients arrive sequentially. These bandit problems became popular with the seminal paper [66], after which they have found applications in diverse fields, such as control, economics, statistics, or learning theory.

Formally, a K-armed bandit problem ($K \geq 2$) is specified by K real-valued distributions. In each time step a decision maker can select one of the distributions to obtain a sample from it. The samples obtained are considered as rewards. The distributions are initially unknown to the decision maker, whose goal is to maximize the sum of the rewards received, or equivalently, to minimize the regret which is defined as the loss compared to the total payoff that can be achieved given full knowledge of the problem, *i.e.*, when the arm giving the highest expected reward is pulled all the time.

The name "bandit" comes from imagining a gambler playing with K slot machines. The gambler can pull the arm of any of the machines, which produces a random payoff as a result: When arm k is pulled, the random payoff is drawn from the distribution associated to k. Since the payoff distributions are initially unknown, the gambler must use exploratory actions to learn the utility of the individual arms. However, exploration has to be carefully controlled since excessive exploration may lead to unnecessary losses. Hence, to play well, the gambler must carefully balance exploration and exploitation. Auer *et al.* [61] introduced the algorithm UCB (Upper Confidence Bounds) that follows what is now called the "optimism in the face of uncertainty principle". Their algorithm works by computing upper confidence bounds for all the arms and then choosing the arm with the highest such bound. They proved that the expected regret of their algorithm increases at most at a logarithmic rate with the number of trials, and that the algorithm achieves the smallest possible regret up to some sub-logarithmic factor (for the considered family of distributions).

3.3. Statistical analysis of time series

Many of the problems of machine learning can be seen as extensions of classical problems of mathematical statistics to their (extremely) non-parametric and model-free cases. Other machine learning problems are founded on such statistical problems. Statistical problems of sequential learning are mainly those that are concerned with the analysis of time series. These problems are as follows.

3.3.1. Prediction of Sequences of Structured and Unstructured Data

Given a series of observations $x_1, \cdots, x_n$ it is required to give forecasts concerning the distribution of the future observations $x_{n+1}, x_{n+2}, \cdots$; in the simplest case, that of the next outcome x_{n+1}. Then x_{n+1} is revealed and the process continues. Different goals can be formulated in this setting. One can either make some assumptions on the probability measure that generates the sequence $x_1, \cdots, x_n, \cdots$, such as that the outcomes are independent and identically distributed (i.i.d.), or that the sequence is a Markov chain, that it is a stationary process, etc. More generally, one can assume that the data is generated by a probability measure that belongs to a certain set $\mathcal{C}$. In these cases the goal is to have the discrepancy between the predicted and the "true" probabilities to go to zero, if possible, with guarantees on the speed of convergence.

Alternatively, rather than making some assumptions on the data, one can change the goal: the predicted probabilities should be asymptotically as good as those given by the best reference predictor from a certain pre-defined set.

Another dimension of complexity in this problem concerns the nature of observations x_i. In the simplest case, they come from a finite space, but already basic applications often require real-valued observations. Moreover, function or even graph-valued observations often arise in practice, in particular in applications concerning Web data. In these settings estimating even simple characteristics of probability distributions of the future outcomes becomes non-trivial, and new learning algorithms for solving these problems are in order.

3.3.2. Hypothesis testing

Given a series of observations of $x_1, \cdots, x_n, \cdots$ generated by some unknown probability measure μ, the problem is to test a certain given hypothesis H_0 about μ, versus a given alternative hypothesis H_1. There are many different examples of this problem. Perhaps the simplest one is testing a simple hypothesis "μ is Bernoulli i.i.d. measure with probability of 0 equals 1/2" versus "μ is Bernoulli i.i.d. with the parameter different from 1/2". More interesting cases include the problems of model verification: for example, testing that μ is a Markov chain, versus that it is a stationary ergodic process but not a Markov chain. In the case when we have not one but several series of observations, we may wish to test the hypothesis that they are independent, or that they are generated by the same distribution. Applications of these problems to a more general class of machine learning tasks include the problem of feature selection, the problem of testing that a certain behaviour (such as pulling a certain arm of a bandit, or using a certain policy) is better (in terms of achieving some goal, or collecting some rewards) than another behaviour, or than a class of other behaviours.

The problem of hypothesis testing can also be studied in its general formulations: given two (abstract) hypothesis H_0 and H_1 about the unknown measure that generates the data, find out whether it is possible to test H_0 against H_1 (with confidence), and if yes then how can one do it.

3.3.3. Change Point Analysis

A stochastic process is generating the data. At some point, the process distribution changes. In the "offline" situation, the statistician observes the resulting sequence of outcomes and has to estimate the point or the points at which the change(s) occurred. In online setting, the goal is to detect the change as quickly as possible.

These are the classical problems in mathematical statistics, and probably among the last remaining statistical problems not adequately addressed by machine learning methods. The reason for the latter is perhaps in that the problem is rather challenging. Thus, most methods available so far are parametric methods concerning piecewise constant distributions, and the change in distribution is associated with the change in the mean. However, many applications, including DNA analysis, the analysis of (user) behaviour data, etc., fail to comply with this kind of assumptions. Thus, our goal here is to provide completely non-parametric methods allowing for any kind of changes in the time-series distribution.

3.3.4. Clustering Time Series, Online and Offline

The problem of clustering, while being a classical problem of mathematical statistics, belongs to the realm of unsupervised learning. For time series, this problem can be formulated as follows: given several samples $x^1 = (x_1^1, \cdots, x_{n_1}^1), \cdots, x^N = (x_N^1, \cdots, x_{n_N}^N)$, we wish to group similar objects together. While this is of course not a precise formulation, it can be made precise if we assume that the samples were generated by k different distributions.

The online version of the problem allows for the number of observed time series to grow with time, in general, in an arbitrary manner.

3.3.5. Online Semi-Supervised Learning

Semi-supervised learning (SSL) is a field of machine learning that studies learning from both labeled and unlabeled examples. This learning paradigm is extremely useful for solving real-world problems, where data is often abundant but the resources to label them are limited.

Furthermore, *online* SSL is suitable for adaptive machine learning systems. In the classification case, learning is viewed as a repeated game against a potentially adversarial nature. At each step t of this game, we observe an example $\mathbf{x_t}$, and then predict its label $\widehat{y}_t$.

The challenge of the game is that we only exceptionally observe the true label y_t. In the extreme case, which we also study, only a handful of labeled examples are provided in advance and set the initial bias of the system while unlabeled examples are gathered online and update the bias continuously. Thus, if we want to adapt to changes in the environment, we have to rely on indirect forms of feedback, such as the structure of data.

3.3.6. Online Kernel and Graph-Based Methods

Large-scale kernel ridge regression is limited by the need to store a large kernel matrix. Similarly, large-scale graph-based learning is limited by storing the graph Laplacian. Furthermore, if the data come online, at some point no finite storage is sufficient and per step operations become slow.

Our challenge is to design sparsification methods that give guaranteed approximate solutions with a reduced storage requirements.

SIERRA Project-Team

3. Research Program

3.1. Supervised Learning

This part of our research focuses on methods where, given a set of examples of input/output pairs, the goal is to predict the output for a new input, with research on kernel methods, calibration methods, and multi-task learning.

3.2. Unsupervised Learning

We focus here on methods where no output is given and the goal is to find structure of certain known types (e.g., discrete or low-dimensional) in the data, with a focus on matrix factorization, statistical tests, dimension reduction, and semi-supervised learning.

3.3. Parsimony

The concept of parsimony is central to many areas of science. In the context of statistical machine learning, this takes the form of variable or feature selection. The team focuses primarily on structured sparsity, with theoretical and algorithmic contributions.

3.4. Optimization

Optimization in all its forms is central to machine learning, as many of its theoretical frameworks are based at least in part on empirical risk minimization. The team focuses primarily on convex and bandit optimization, with a particular focus on large-scale optimization.

SPHINX Project-Team

3. Research Program

3.1. Control and stabilization of heterogeneous systems

Fluid-Structure Interaction Systems (FSIS) are present in many physical problems and applications. Their study involves to solve several challenging mathematical problems:

- **Nonlinearity:** One has to deal with a system of nonlinear PDE such as the Navier-Stokes or the Euler systems;
- **Coupling:** The corresponding equations couple two systems of different types and the methods associated with each system need to be suitably combined to solve successfully the full problem;
- **Coordinates:** The equations for the structure are classically written with Lagrangian coordinates whereas the equations for the fluid are written with Eulerian coordinates;
- **Free boundary:** The fluid domain is moving and its motion depends on the motion of the structure. The fluid domain is thus an unknown of the problem and one has to solve a free boundary problem.

In order to control such FSIS systems, one has first to analyze the corresponding system of PDE. The oldest works on FSIS go back to the pioneering contributions of Thomson, Tait and Kirchhoff in the 19th century and Lamb in the 20th century, who considered simplified models (potential fluid or Stokes system). The first mathematical studies in the case of a viscous incompressible fluid modeled by the Navier-Stokes system and a rigid body whose dynamics is modeled by Newton's laws appeared much later [108], [100], [79], and almost all mathematical results on such FSIS have been obtained in the last twenty years.

The most studied issue concerns the well-posedness of the problem modeling a **rigid body moving into a viscous incompressible fluid**. If the fluid fills the **unbounded domain** surrounding the structure, the free boundary difficulty can be overcome by using a simple change of variables that makes the rigid body fixed. One can then use classical tools for the Navier-Stokes system and obtain the existence of weak solutions (see, for instance, [67], [68], [101]) or strong solutions for the case of a ball [105]. When the rigid body is not a ball, the additional terms due to the change of variables modify the nature of the system and only partial results are available for strong solutions [69], [54], [102]. When the fluid-solid system is confined in a **bounded domain**, the above strategy fails. Several papers have developed interesting strategies in order to obtain the existence of solutions. Since the coupling is strong, it is natural to consider a variational formulation for both the fluid and the structure equations (see [57]). One can then solve the FSIS by considering the Navier-Stokes system with a penalization term taking into account the structure ([51], [99], [63]) or using a time discretization in order to fix the rigid body during some time interval ([73]). Using an appropriate change of variables has also been used (see [72], [104]), but of course, its construction is more complex than in the case where the FSIS fills the whole space. Most of the above results only hold up to a possible contact between two structures or between a structure and the exterior boundary. If the considered configuration excludes contacts, some authors also investigated the long-time behavior of this system and the existence of time periodic solutions [107], [89], [70].

Many other FSIS have been studied as well. Let us mention, for instance, **rigid bodies immersed in an incompressible perfect fluid** ([91], [76], [71]), **in a viscous compressible fluid** ([56], [44], [62], [45]), in a **viscous multipolar fluid** or in an **incompressible non-Newtonian fluid** ([64]). The case of **deformable structures** has also been considered, either for a fluid inside a moving structure (e.g. blood motion in arteries) or for a moving deformable structure immersed in a fluid (e.g. fish locomotion). Several models for the dynamics of the deformable structure exist: one can use the plate equations or the elasticity equations. The obtained coupled FSIS is a complex system and the study of its well-posedness raises several difficulties. The main one comes from the fact that we gather two systems of different nature, as the linearized problem couples a parabolic system with a hyperbolic one. Theoretical studies have been performed for approximations of the complete system, using two strategies: adding a regularizing term in the linear elasticity equations (see [49], [44], [82]) or approximate the equations of linear elasticity by a system of finite dimension (see [58], [47]). For strong solutions, the coupling between hyperbolic-parabolic systems leads to seek solutions with high regularity. The only known results [52], [53] in this direction concern local (in time) existence of regular solutions, under strong assumptions on the regularity of the initial data. Such assumptions are not very satisfactory but seem inherent in this coupling between two systems of different natures. Another option is to consider approximate models, but so far, the available approximations are not obtained from a physical model and deriving a more realistic model is a difficult task.

In some particular important physical situations, one can also consider a simplified model. For instance, in order to study self-propelled motions of structures in a fluid, like fish locomotion, one can assume that the **deformation of the structure is prescribed and known**, whereas its displacement remains unknown ([97]). Although simplified, this model already contains many difficulties and permits to start the mathematical study of a challenging problem: understanding the locomotion mechanism of aquatic animals.

Using the above results and the corresponding tools, we aim to consider control or stabilization problems for FSIS. Some control problems have already been considered: using an interior control in the fluid region, it is possible to control locally the velocity of the fluid together with the velocity and the position of the rigid body (see [77], [46]). The strategy of control is similar to the classical method for a fluid (without solid) (see, for instance, [65]) but with the tools developed in [104]. A first result of stabilization was obtained in [93] and concerns a fluid contained in bounded cavity where a part of the boundary is modeled by a plate system. The feedback control is a force applied on the whole plate and it allows the author to obtain a local stabilization result around the null state.

To extend these first results of control and stabilization, we first have to make some progress in the analysis of FSIS:

- **Contact:** It is important to understand the behavior of the system when two structures are close, and in particular to understand how to deal with contact problems;
- **Deformable structures:** To handle such structures, we need to develop new ideas and techniques in order to couple two dynamics of infinite dimension and of different nature.

At the same time, we can tackle control problems for simplified models. For instance, in some regimes, the Navier-Stokes system can be replaced by the Stokes system and the Euler system by Laplace's equation

3.2. Inverse problems for heterogeneous systems

The area of inverse problems covers a large class of theoretical and practical issues which are important in many applications (see for instance the books of Isakov [78] or Kaltenbacher, Neubauer, and Scherzer [80]). Roughly speaking, an inverse problem is a problem where one attempts to recover an unknown property of a given system from its response to an external probing signal. For systems described by evolution PDE, one can be interested in the reconstruction from partial measurements of the state (initial, final or current), the inputs (a source term, for instance) or the parameters of the model (a physical coefficient for example). For stationary or periodic problems (i.e. problems where the time dependence is given), one can be interested in determining from boundary data a local heterogeneity (shape of an obstacle, value of a physical coefficient describing the medium, etc.). Such inverse problems are known to be generally ill-posed and their study leads to investigate the following questions:

- *Uniqueness.* The question here is to know whether the measurements uniquely determine the unknown quantity to be recovered. This theoretical issue is a preliminary step in the study of any inverse problem and can be a hard task.
- *Stability.* When uniqueness is ensured, the question of stability, which is closely related to sensitivity, deserves special attention. Stability estimates provides an upper bound for the parameter error given some uncertainty on data. This issue is closely related to the so-called observability inequality in systems theory.

- *Reconstruction.* Inverse problems being usually ill-posed, one needs to develop specific reconstruction algorithms which are robust with respect to noise, disturbances and discretization. A wide class of methods is based on optimization techniques.

In this project, we investigate two classes of inverse problems, which both appear in FSIS and CWS:

1. **Identification for evolution PDE.**

   Driven by applications, the identification problem for systems of infinite dimension described by evolution PDE has known in the last three decades a fast and significant growth. The unknown to be recovered can be the (initial/final) state (e.g. state estimation problems [38], [66], [74], [103] for the design feedback controllers), an input (for instance source inverse problems [35], [48], [59]) or a parameter of the system. These -linear or non linear- problems are generally ill-posed and many regularization approaches have been developed. Among the different methods used for identification, let us mention optimization techniques ([50]), specific one-dimensional techniques (like in [39]) or observer-based methods as in [87].

   In the last few years, we have developed observers to solve initial data inverse problems for a class of linear systems of infinite dimension and of the form $\dot{z}(t) = Az(t)$ (A denotes here the generator of a C_0 semigroup) from an output $y(t) = Cz(t)$ measured through a finite time interval. Let us recall that observers (or Luenberger observers [86]) have been introduced in automatic control theory to estimate the state of a dynamical system (of finite dimension) from the knowledge of an output (and, of course, assuming that the initial state is unknown). Roughly speaking, an observer is an auxiliary dynamical system that uses as inputs the available measurements (that is the output of the original system) that converges asymptotically (in time) towards the state of the original system. Observers are very popular in the community of automatic control and have given rise to a wide literature (for more references, see for instance the book by O'Reilly [90] and more recently the one by Trinh and Fernando [106] devoted to functional observers). The generalization of observers (also called estimators or filters in the stochastic framework) to systems of infinite dimension goes back to the seventies (see for instance Bensoussan [42] or Curtain and Zwart [55]) and the theory is definitely less developed than in the case of finite dimension . Using observers, we have proposed in [92], [75] an iterative algorithm to reconstruct initial data from partial measurements for some evolution equations, including the wave and Schrödinger systems (and more generally for skew-adjoint generators). This algorithm also provides a new method to solve source inverse problems, in the case where the source term has a specific structure (separate variables in time-space with known time dependence). We are deepening our activities in this direction by considering more general operators or more general sources and the reconstruction of coefficients for the wave equation. In connection with this last problem, we study the stability in the determination of these coefficients. To achieve this, we use geometrical optics, which is a classical albeit powerful tool to obtain quantitative stability estimates on some inverse problems with a geometrical background, see for instance [41], [40].

2. **Geometric inverse problems.**

   We investigate some geometric inverse problems that appear naturally in many applications, like medical imaging and non destructive testing. A typical problem we have in mind is the following: given a domain Ω containing an (unknown) local heterogeneity ω, we consider the boundary value problem of the form

$$\begin{cases} Lu = 0, & (\Omega \setminus \omega) \\ u = f, & (\partial\Omega) \\ Bu = 0, & (\partial\omega) \end{cases}$$

where L is a given partial differential operator describing the physical phenomenon under consideration (typically a second order differential operator), B the (possibly unknown) operator describing the boundary condition on the boundary of the heterogeneity and f the exterior source used to probe the medium. The question is then to recover the shape of ω and/or the boundary operator B from some measurement Mu on the outer boundary $\partial\Omega$. This setting includes in particular inverse scattering problems in acoustics and electromagnetics (in this case Ω is the whole space and the data are far field measurements) and the inverse problem of detecting solids moving in a fluid. It also includes, with slight modifications, more general situations of incomplete data (i.e. measurements on part of the outer boundary) or penetrable inhomogeneities. Our approach to tackle this type of problems is based on the derivation of a series expansion of the input-to-output map of the problem (typically the Dirchlet-to-Neumann map of the problem for the Calderón problem) in terms of the size of the obstacle.

3.3. Numerical analysis and simulation of heterogeneous systems

Within the team, we have developed in the last few years numerical codes for the simulation of FSIS and CWS. We plan to continue our efforts in this direction.

- In the case of FSIS, our main objective is to provide computational tools for the scientific community, essentially to solve academic problems.
- In the case of CWS, our main objective is to build tools general enough to handle industrial problems. Our strong collaboration with Christophe Geuzaine's team in Liege (Belgium) makes this objective credible, through the combination of DDM (Domain Decomposition Methods) and parallel computing.

Below, we explain in detail the corresponding scientific program.

- **Simulation of FSIS:** In order to simulate fluid-structure systems, one has to deal with the fact that the fluid domain is moving and that the two systems for the fluid and for the structure are strongly coupled. To overcome this free boundary problem, three main families of methods are usually applied to numerically compute in an efficient way the solutions of the fluid-structure interaction systems. The first method consists in suitably displacing the mesh of the fluid domain in order to follow the displacement and the deformation of the structure. A classical method based on this idea is the A.L.E. (Arbitrary Lagrangian Eulerian) method: with such a procedure, it is possible to keep a good precision at the interface between the fluid and the structure. However, such methods are difficult to apply for large displacements (typically the motion of rigid bodies). The second family of methods consists in using a *fixed mesh* for both the fluid and the structure and to simultaneously compute the velocity field of the fluid with the displacement velocity of the structure. The presence of the structure is taken into account through the numerical scheme. There are several methods in that direction: immersed boundary method, fictitious domain method, fat boundary method, the Lagrange-Galerkin method. Finally, the third class of methods consists in transforming the set of PDEs governing the flow into a system of integral equations set on the boundary of the immersed structure. Thus, only the surface of the structure is meshed and this mesh moves along with the structure. Notice that this method can be applied only for the flow of particular fluids (ideal fluid or stationary Stokes flow).

  The members of SPHINX have already worked on these three families of numerical methods for FSIS systems with rigid bodies (see e.g. [96], [81], [98], [94], [95], [88]). We plan to work on numerical methods for FSIS systems with non-rigid structures immersed into an incompressible viscous fluid. In particular, we will focus our work on the development and the analysis of numerical schemes and, on the other hand, on the efficient implementation of the corresponding numerical methods.
- **Simulation of CWS:** Solving acoustic or electromagnetic scattering problems can become a tremendously hard task in some specific situations. In the high frequency regime (i.e. for small wavelength),

acoustic (Helmholtz's equation) or electromagnetic (Maxwell's equations) scattering problems are known to be difficult to solve while being crucial for industrial applications (e.g. in aeronautics and aerospace engineering). Our particularity is to develop new numerical methods based on the hybridization of standard numerical techniques (like algebraic preconditioners, etc.) with approaches borrowed from asymptotic microlocal analysis. Most particularly, we contribute to building hybrid algebraic/analytical preconditioners and quasi-optimal Domain Decomposition Methods (DDM) [43], [60], [61] for highly indefinite linear systems. Corresponding three-dimensional solvers (like for example GetDDM) will be developed and tested on realistic configurations (e.g. submarines, complete or parts of an aircraft, etc.) provided by industrial partners (Thales, Airbus). Another situation where scattering problems can be hard to solve is the one of dense multiple (acoustic, electromagnetic or elastic) scattering media. Computing waves in such media requires to take into account not only the interaction between the incident wave and the scatterers, but also the effects of the interactions between the scatterers themselves. When the number of scatterers is very large (and possibly for high frequency [37], [36]), specific deterministic or stochastic numerical methods and algorithms are needed. We introduce new optimized numerical methods for solving such complex configurations. Many applications are related to this kind of problem like e.g. for osteoporosis diagnosis where quantitative ultrasound is a recent and promising technique to detect a risk of fracture. Therefore, numerical simulation of wave propagation in multiple scattering elastic medium in the high frequency regime is a very useful tool for this purpose.

TAO Project-Team

3. Research Program

3.1. The Five Pillars of TAO

This Section describes TAO main research directions at the crossroad of Machine Learning and Evolutionary Computation. Since 2008, TAO has been structured in several special interest groups (SIGs) to enable the agile investigation of long-term or emerging theoretical and applicative issues. The comparatively small size of TAO SIGs enables in-depth and lively discussions; the fact that all TAO members belong to several SIGs, on the basis of their personal interests, enforces the strong and informal collaboration of the groups, and the fast information dissemination.

The first two SIGs consolidate the key TAO scientific pillars, while the others evolve and adapt to new topics.

The **Stochastic Continuous Optimization** SIG (OPT-SIG) takes advantage of the fact that TAO is acknowledged the best French research group and one of the top international groups in evolutionary computation from a theoretical and algorithmic standpoint. A main priority on the OPT-SIG research agenda is to provide theoretical and algorithmic guarantees for the current world state-of-the-art continuous stochastic optimizer, CMA-ES, ranging from convergence analysis to a rigorous benchmarking methodology. Incidentally, the benchmark platform COCO has been acknowledged since 2009 as “the“ international continuous optimization benchmark, and its extension is at the core of the ANR projects NumBBO and NumBBO2. Another priority is to address the current limitations of CMA-ES in terms of high-dimensional or expensive optimization and constraint handling (respectively Ouassim Ait El Hara’s and Asma Atamna’s PhDs). Note that most members of this SIG have moved to the recently created Inria team RANDOPT by December 2016.

The **Optimal Decision Making under Uncertainty** SIG (UCT-SIG) benefits from the MoGo expertise and its past and present world records in the domain of computer-Go, establishing the international visibility of TAO in sequential decision making. Since 2010, UCT-SIG resolutely moves to address the problems of **energy management** from a fundamental and applied perspective. On the one hand, energy management offers a host of challenging issues, ranging from long-horizon policy optimization to the combinatorial nature of the search space, from the modeling of prior knowledge to non-stationary environment to name a few. On the other hand, the energy management issue can hardly be tackled in a pure academic perspective: tight collaborations with industrial partners are needed to access the true operational constraints. Such international and national collaborations have been started by Olivier Teytaud during his three stays (1 year, 6 months, 6 months) in Taiwan, and witnessed by the FP7 STREP Citines, the ADEME Post contract, and the METIS I-lab with SME Artelys. Note that Olivier Teytaud has left TAO for Google-Zurich on June 6., 2016. The project is continuing in collaboration with RTE under the leadership of Isabelle Guyon and Marc Schoenauer, making connections with Data Science.

The **Data Science** SIG (DS-SIG) includes the activities conducted or started within the CDS and ISN Lidexes in Saclay. On the one hand, it replaces and extends the former *Distributed systems* SIG, that was devoted to the modeling and optimization of (large scale) distributed systems, and itself was extending the goals of the original *Autonomic Computing* SIG, initiated by Cécile Germain-Renaud and investigating the use of statistical Machine Learning for large scale computational architectures (from data acquisition – the Grid Observatory in the European Grid Initiative – to grid management and fault detection). Under the application pressure from natural and social sciences (ranging from High Energy Physics to computational social sciences), this SIG has evolved. A major result of this theme has been the creation 3 years ago of the Paris-Saclay Center for Data Science, co-chaired by Balázs Kégl, and the organization of the Higgs-ML challenge (http://higgsml.lal.in2p3.fr/), most popular challenge ever on the Kaggle platform. Another large scale data challenge sponsored by Microsoft with USD 60000 in prizes on the theme of Automatic Machine Learning (AutoML) in 2015/2016 was crowned by success: the winners developed a new tool called AutoSKlearn as a wrapper to the scikit-learn library, an open source project lead by Inria team Parietal.

On the other hand, several activities around Computational Social Sciences involving Gregory Grefenstette, Cécile Germain-Renaud, Michèle Sebag, Philippe Caillou, Isabelle Guyon and Paola Tubaro, have widely extended previous work around the modeling of multi-agent systems and the exploitation of simulation results in the SimTools RNSC network frame. A research direction involves adding semantics to underspecified collections of societal information: in an historical perspective (as in the new TAO H2020 project, EHRI-II on holocaust archives, or in the Gregorius project on church history) or an individual perspective (as in the ongoing Personal Semantics project). Another research direction, developed within the Paris-Saclay Institute for Digital Society (ISN Lidex), examines societal questions (frictional unemployment, Th. Schmitt's PhD, or quality of life at work, O. Goudet's post-doc, or scientific institution activities, F. Louistisserand's engineer stint on Cartolabe) in a data-driven perspective. The key challenge here is to use learning algorithms to find structure and extract knowledge from poorly structured or unstructured information, and to provide intelligible results and/or means to interact with the user. Novel approaches involving causal modeling are under exploration.

The **Designing Criteria** SIG (CRI-SIG) focuses on the design of learning and optimization criteria. It elaborates on the lessons learned from the former *Complex Systems* SIG, showing that the key issue in challenging applications often is to design the objective itself. Such targeted criteria are pervasive in the study and building of autonomous cognitive systems, ranging from intrinsic rewards in robotics to the notion of saliency in vision and image understanding, and that of automatic algorithm selection and parameterization. The desired criteria can also result from fundamental requirements, such as scale invariance in a statistical physics perspective, and guide the algorithmic design. Additionally, the criteria can also be domain-driven and reflect the expert priors concerning the structure of the sought solution (e.g., spatio-temporal consistency); the challenge is to formulate such criteria in a mixed non convex/non differentiable objective function, nevertheless amenable to tractable optimization.

The **Deep Learning and Information Theory** SIG (DEEP-SIG) originated from some extensions of the work done in the *Distributed Systems* SIG that have been developped in the context of the TIMCO FUI project (started end 2012 and just ended); the challenge was not only to port ML algorithms on massively distributed architectures, but to see how these architectures can inspire new ML criteria and methodologies. The coincidence of this project with the arrival of Yann Ollivier in TAO gradualy led this work toward Deep Networks. Other research themes of this SIG are concerned with studying various theoretical and practical aspects of deep learning, providing information-theoretic perspectives on the design and optimization of deep learning models, such as using the Fisher information matrix to optimize the parameters, or using minimum description length criteria to choose the right model structure (topology of the neural graph, addition or removal of parameters...) and to provide regularization and model selection. This activity has also branched out into exploring various applications of Deep Learning. Isabelle Guyon has been involved in applications in computer vision, including the study of personality traits in video data and the verification of fingerprints. Energy Management (Section 4.1), Computational Social Sciences (Section 4.2), and anomaly detection are now also steered toward using Deep Networks for different variants of representation learning.

TOSCA Project-Team

3. Research Program

3.1. Research Program

Most often physicists, economists, biologists and engineers need a stochastic model because they cannot describe the physical, economical, biological, etc., experiment under consideration with deterministic systems, either because of its complexity and/or its dimension or because precise measurements are impossible. Therefore, they abandon trying to get the exact description of the state of the system at future times given its initial conditions, and try instead to get a statistical description of the evolution of the system. For example, they desire to compute occurrence probabilities for critical events such as the overstepping of a given thresholds by financial losses or neuronal electrical potentials, or to compute the mean value of the time of occurrence of interesting events such as the fragmentation to a very small size of a large proportion of a given population of particles. By nature such problems lead to complex modelling issues: one has to choose appropriate stochastic models, which require a thorough knowledge of their qualitative properties, and then one has to calibrate them, which requires specific statistical methods to face the lack of data or the inaccuracy of these data. In addition, having chosen a family of models and computed the desired statistics, one has to evaluate the sensitivity of the results to the unavoidable model specifications. The TOSCA team, in collaboration with specialists of the relevant fields, develops theoretical studies of stochastic models, calibration procedures, and sensitivity analysis methods.

In view of the complexity of the experiments, and thus of the stochastic models, one cannot expect to use closed form solutions of simple equations in order to compute the desired statistics. Often one even has no other representation than the probabilistic definition (e.g., this is the case when one is interested in the quantiles of the probability law of the possible losses of financial portfolios). Consequently the practitioners need Monte Carlo methods combined with simulations of stochastic models. As the models cannot be simulated exactly, they also need approximation methods which can be efficiently used on computers. The TOSCA team develops mathematical studies and numerical experiments in order to determine the global accuracy and the global efficiency of such algorithms.

The simulation of stochastic processes is not motivated by stochastic models only. The stochastic differential calculus allows one to represent solutions of certain deterministic partial differential equations in terms of probability distributions of functionals of appropriate stochastic processes. For example, elliptic and parabolic linear equations are related to classical stochastic differential equations (SDEs), whereas nonlinear equations such as the Burgers and the Navier–Stokes equations are related to McKean stochastic differential equations describing the asymptotic behavior of stochastic particle systems. In view of such probabilistic representations one can get numerical approximations by using discretization methods of the stochastic differential systems under consideration. These methods may be more efficient than deterministic methods when the space dimension of the PDE is large or when the viscosity is small. The TOSCA team develops new probabilistic representations in order to propose probabilistic numerical methods for equations such as conservation law equations, kinetic equations, and nonlinear Fokker–Planck equations.

TROPICAL Team

3. Research Program

3.1. Optimal control and zero-sum games

The dynamic programming approach allows one to analyze one or two-player dynamic decision problems by means of operators, or partial differential equations (Hamilton–Jacobi or Isaacs PDEs), describing the time evolution of the value function, i.e., of the optimal reward of one player, thought of as a function of the initial state and of the horizon. We work especially with problems having long or infinite horizon, modelled by stopping problems, or ergodic problems in which one optimizes a mean payoff per time unit. The determination of optimal strategies reduces to solving nonlinear fixed point equations, which are obtained either directly from discrete models, or after a discretization of a PDE.

The geometry of solutions of optimal control and game problems Basic questions include, especially for stationary or ergodic problems, the understanding of existence and uniqueness conditions for the solutions of dynamic programming equations, for instance in terms of controllability or ergodicity properties, and more generally the understanding of the structure of the full set of solutions of stationary Hamilton–Jacobi PDEs and of the set of optimal strategies. These issues are already challenging in the one-player deterministic case, which is an application of choice of tropical methods, since the Lax-Oleinik semigroup, i.e., the evolution semigroup of the Hamilton-Jacobi PDE, is a linear operator in the tropical sense. Recent progress in the deterministic case has been made by combining dynamical systems and PDE techniques (weak KAM theory [79]), and also using metric geometry ideas (abstract boundaries can be used to represent the sets of solutions [90], [4]). The two player case is challenging, owing to the lack of compactness of the analogue of the Lax-Oleinik semigroup and to a richer geometry. The conditions of solvability of ergodic problems for games (for instance, solvability of ergodic Isaacs PDEs), and the representation of solutions are only understood in special cases, for instance in the finite state space case, through tropical geometry and non-linear Perron-Frobenius methods [54],[47], [14].

Algorithmic aspects: from combinatorial algorithms to the attenuation of the curse of dimensionality Our general goal is to push the limits of solvable models by means of fast algorithms adapted to large scale instances. Such instances arise from discrete problems, in which the state space may so large that it is only accessible through local oracles (for instance, in some web ranking applications, the number of states may be the number of web pages) [80]. They also arise from the discretization of PDEs, in which the number of states grows exponentially with the number of degrees of freedom, according to the “curse of dimensionality”. A first line of research is the development of *new approximation methods for the value function*. So far, classical approximations by linear combinations have been used, as well as approximation by suprema of linear or quadratic forms, which have been introduced in the setting of dual dynamic programming and of the so called “max-plus basis methods” [81]. We believe that more concise or more accurate approximations may be obtained by unifying these methods. Also, some max-plus basis methods have been shown to *attenuate the curse of dimensionality* for very special problems (for instance involving switching) [98], [84]. This suggests that the complexity of control or games problems may be measured by more subtle quantities that the mere number of states, for instance, by some forms of metric entropy (for example, certain large scale problems have a low complexity owing to the presence of decomposition properties, “highway hierarchies”, etc.). A second line of of our research is the development of *combinatorial algorithms*, to solve large scale zero-sum two-player problems with discrete state space. This is related to current open problems in algorithmic game theory. In particular, the existence of polynomial-time algorithms for games with ergodic payment is an open question. See e.g. [5] for a polynomial time average complexity result derived by tropical methods. The two lines of research are related, as the understanding of the geometry of solutions allows to develop better approximation or combinatorial algorithms.

3.2. Non-linear Perron-Frobenius theory, nonexpansive mappings and metric geometry

Several applications (including population dynamics [9] and discrete event systems [66], [71], [62]) lead to studying classes of dynamical systems with remarkable properties: preserving a cone, preserving an order, or being nonexpansive in a metric. These can be studied by techniques of non-linear Perron-Frobenius theory [14] or metric geometry [10]. Basic issues concern the existence and computation of the "escape rate" (which determines the throughput, the growth rate of the population), the characterizations of stationary regimes (non-linear fixed points), or the study of the dynamical properties (convergence to periodic orbits). Nonexpansive mappings also play a key role in the "operator approach" to zero-sum games, since the one-day operators of games are nonexpansive in several metrics, see [8].

3.3. Tropical algebra and convex geometry

The different applications mentioned in the other sections lead us to develop some basic research on tropical algebraic structures and in convex and discrete geometry, looking at objects or problems with a "piecewise-linear " structure. These include the geometry and algorithmics of tropical convex sets [64], [56], tropical semialgebraic sets [49], the study of semi-modules (analogues of vector spaces when the base field is replaced by a semi-field), the study of systems of equations linear in the tropical sense, investigating for instance the analogues of the notions of rank, the analogue of the eigenproblems [15], and more generally of systems of tropical polynomial equations. Our research also builds on, and concern, classical convex and discrete geometry methods.

3.4. Tropical methods applied to optimization, perturbation theory and matrix analysis

Tropical algebraic objects appear as a deformation of classical objects thought various asymptotic procedures. A familiar example is the rule of asymptotic calculus,

$$e^{-a/\epsilon}+e^{-b/\epsilon}\asymp e^{-\min(a,b)/\epsilon}\enspace ,\qquad e^{-a/\epsilon}\times e^{-b/\epsilon}=e^{-(a+b)/\epsilon}\enspace , \tag{69}$$

when $\epsilon\to 0^+$. Deformations of this kind have been studied in different contexts: large deviations, zero-temperature limits, Maslov's "dequantization method" [97], non-archimedean valuations, log-limit sets and Viro's patchworking method [116], etc.

This entails a relation between classical algorithmic problems and tropical algorithmic problems, one may first solve the $\epsilon=0$ case (non-archimedean problem), which is sometimes easier, and then use the information gotten in this way to solve the $\epsilon=1$ (archimedean) case.

In particular, tropicalization establishes a connection between polynomial systems and piecewise affine systems that are somehow similar to the ones arising in game problems. It allows one to transfer results from the world of combinatorics to "classical" equations solving. We investigate the consequences of this correspondence on complexity and numerical issues. For instance, combinatorial problems can be solved in a robust way. Hence, situations in which the tropicalization is faithful lead to improved algorithms for classical problems. In particular, scalings for the polynomial eigenproblems based on tropical preprocessings have started to be used in matrix analysis [85], [88].

Moreover, the tropical approach has been recently applied to construct examples of linear programs in which the central path has an unexpectedly high total curvature [61], and it has also led to positive polynomial-time average case results concerning the complexity of mean payoff games. Similarly, we are studying semidefinite programming over non-archimedean fields [49], [29], with the goal to better understand complexity issues in classical semidefinite and semi-algebraic programming.

ABS Project-Team

3. Research Program

3.1. Introduction

The research conducted by ABS focuses on three main directions in Computational Structural Biology (CSB), together with the associated methodological developments:
– Modeling interfaces and contacts,
– Modeling macro-molecular assemblies,
– Modeling the flexibility of macro-molecules,
– Algorithmic foundations.

3.2. Modeling interfaces and contacts

Keywords: Docking, interfaces, protein complexes, structural alphabets, scoring functions, Voronoi diagrams, arrangements of balls.

The Protein Data Bank, http://www.rcsb.org/pdb, contains the structural data which have been resolved experimentally. Most of the entries of the PDB feature isolated proteins [0], the remaining ones being protein - protein or protein - drug complexes. These structures feature what Nature does – up to the bias imposed by the experimental conditions inherent to structure elucidation, and are of special interest to investigate non-covalent contacts in biological complexes. More precisely, given two proteins defining a complex, interface atoms are defined as the atoms of one protein *interacting* with atoms of the second one. Understanding the structure of interfaces is central to understand biological complexes and thus the function of biological molecules [48]. Yet, in spite of almost three decades of investigations, the basic principles guiding the formation of interfaces and accounting for its stability are unknown [51]. Current investigations follow two routes. From the experimental perspective [34], directed mutagenesis enables one to quantify the energetic importance of residues, important residues being termed *hot* residues. Such studies recently evidenced the *modular* architecture of interfaces [45]. From the modeling perspective, the main issue consists of guessing the hot residues from sequence and/or structural informations [40].

The description of interfaces is also of special interest to improve *scoring functions*. By scoring function, two things are meant: either a function which assigns to a complex a quantity homogeneous to a free energy change [0], or a function stating that a complex is more stable than another one, in which case the value returned is a score and not an energy. Borrowing to statistical mechanics [29], the usual way to design scoring functions is to mimic the so-called potentials of mean force. To put it briefly, one reverts Boltzmann's law, that is, denoting $p_i(r)$ the probability of two atoms –defining type i– to be located at distance r, the (free) energy assigned to the pair is computed as $E_i(r) = -kT \log p_i(r)$. Estimating from the PDB one function $p_i(r)$ for each type of pair of atoms, the energy of a complex is computed as the sum of the energies of the pairs located within a distance threshold [49], [36]. To compare the energy thus obtained to a reference state, one may compute $E = \sum_i p_i \log p_i/q_i$, with p_i the observed frequencies, and q_i the frequencies stemming from an a priori model [41]. In doing so, the energy defined is nothing but the Kullback-Leibler divergence between the distributions $\{p_i\}$ and $\{q_i\}$.

Describing interfaces poses problems in two settings: static and dynamic.

[0] For structures resolved by crystallography, the PDB contains the asymmetric unit of the crystal. Determining the biological unit from the asymmetric unit is a problem in itself.

[0] The Gibbs free energy of a system is defined by $G = H - TS$, with $H = U + PV$. G is minimum at an equilibrium, and differences in G drive chemical reactions.

In the static setting, one seeks the minimalist geometric model providing a relevant bio-physical signal. A first step in doing so consists of identifying interface atoms, so as to relate the geometry and the bio-chemistry at the interface level [12]. To elaborate at the atomic level, one seeks a structural alphabet encoding the spatial structure of proteins. At the side-chain and backbone level, an example of such alphabet is that of [30]. At the atomic level and in spite of recent observations on the local structure of the neighborhood of a given atom [50], no such alphabet is known. Specific important local conformations are known, though. One of them is the so-called dehydron structure, which is an under-desolvated hydrogen bond – a property that can be directly inferred from the spatial configuration of the C_α carbons surrounding a hydrogen bond [33].

In the dynamic setting, one wishes to understand whether selected (hot) residues exhibit specific dynamic properties, so as to serve as anchors in a binding process [44]. More generally, any significant observation raised in the static setting deserves investigations in the dynamic setting, so as to assess its stability. Such questions are also related to the problem of correlated motions, which we discuss next.

3.3. Modeling macro-molecular assemblies

Keywords: Macro-molecular assembly, reconstruction by data integration, proteomics, modeling with uncertainties, curved Voronoi diagrams, topological persistence.

3.3.1. Reconstruction by Data Integration

Large protein assemblies such as the Nuclear Pore Complex (NPC), chaperonin cavities, the proteasome or ATP synthases, to name a few, are key to numerous biological functions. To improve our understanding of these functions, one would ideally like to build and animate atomic models of these molecular machines. However, this task is especially tough, due to their size and their plasticity, but also due to the flexibility of the proteins involved. In a sense, the modeling challenges arising in this context are different from those faced for binary docking, and also from those encountered for intermediate size complexes which are often amenable to a processing mixing (cryo-EM) image analysis and classical docking. To face these new challenges, an emerging paradigm is that of reconstruction by data integration [28]. In a nutshell, the strategy is reminiscent from NMR and consists of mixing experimental data from a variety of sources, so as to find out the model(s) best complying with the data. This strategy has been in particular used to propose plausible models of the Nuclear Pore Complex [27], the largest assembly known to date in the eukaryotic cell, and consisting of 456 protein *instances* of 30 *types*.

3.3.2. Modeling with Uncertainties and Model Assessment

Reconstruction by data integration requires three ingredients. First, a parametrized model must be adopted, typically a collection of balls to model a protein with pseudo-atoms. Second, as in NMR, a functional measuring the agreement between a model and the data must be chosen. In [26], this functional is based upon *restraints*, namely penalties associated to the experimental data. Third, an optimization scheme must be selected. The design of restraints is notoriously challenging, due to the ambiguous nature and/or the noise level of the data. For example, Tandem Affinity Purification (TAP) gives access to a *pullout* i.e. a list of protein types which are known to interact with one tagged protein type, but no information on the number of complexes or on the stoichiometry of proteins types within a complex is provided. In cryo-EM, the envelope enclosing an assembly is often imprecisely defined, in particular in regions of low density. For immuno-EM labelling experiments, positional uncertainties arise from the microscope resolution.

These uncertainties coupled with the complexity of the functional being optimized, which in general is non convex, have two consequences. First, it is impossible to single out a unique reconstruction, and a set of plausible reconstructions must be considered. As an example, 1000 plausible models of the NPC were reported in [26]. Interestingly, averaging the positions of all balls of a particular protein type across these models resulted in 30 so-called *probability density maps*, each such map encoding the probability of presence of a particular protein type at a particular location in the NPC. Second, the assessment of all models (individual and averaged) is non trivial. In particular, the lack of straightforward statistical analysis of the individual models and the absence of assessment for the averaged models are detrimental to the mechanistic exploitation of the reconstruction results. At this stage, such models therefore remain qualitative.

3.4. Modeling the flexibility of macro-molecules

Keywords: Folding, docking, energy landscapes, induced fit, molecular dynamics, conformers, conformer ensembles, point clouds, reconstruction, shape learning, Morse theory.

Proteins in vivo vibrate at various frequencies: high frequencies correspond to small amplitude deformations of chemical bonds, while low frequencies characterize more global deformations. This flexibility contributes to the entropy thus the `free energy` of the system *protein - solvent*. From the experimental standpoint, NMR studies generate ensembles of conformations, called `conformers`, and so do molecular dynamics (MD) simulations. Of particular interest while investigating flexibility is the notion of correlated motion. Intuitively, when a protein is folded, all atomic movements must be correlated, a constraint which gets alleviated when the protein unfolds since the steric constraints get relaxed [0]. Understanding correlations is of special interest to predict the folding pathway that leads a protein towards its native state. A similar discussion holds for the case of partners within a complex, for example in the third step of the *diffusion - conformer selection - induced fit* complex formation model.

Parameterizing these correlated motions, describing the corresponding energy landscapes, as well as handling collections of conformations pose challenging algorithmic problems.

At the side-chain level, the question of improving rotamer libraries is still of interest [32]. This question is essentially a clustering problem in the parameter space describing the side-chains conformations.

At the atomic level, flexibility is essentially investigated resorting to methods based on a classical potential energy (molecular dynamics), and (inverse) kinematics. A molecular dynamics simulation provides a point cloud sampling the conformational landscape of the molecular system investigated, as each step in the simulation corresponds to one point in the parameter space describing the system (the conformational space) [47]. The standard methodology to analyze such a point cloud consists of resorting to normal modes. Recently, though, more elaborate methods resorting to more local analysis [43], to Morse theory [38] and to analysis of meta-stable states of time series [39] have been proposed.

3.5. Algorithmic foundations

Keywords: Computational geometry, computational topology, optimization, data analysis.

Making a stride towards a better understanding of the biophysical questions discussed in the previous sections requires various methodological developments, which we briefly discuss now.

3.5.1. Modeling Interfaces and Contacts

In modeling interfaces and contacts, one may favor geometric or topological information.

On the geometric side, the problem of modeling contacts at the atomic level is tantamount to encoding multi-body relations between an atom and its neighbors. On the one hand, one may use an encoding of neighborhoods based on geometric constructions such as Voronoi diagrams (affine or curved) or arrangements of balls. On the other hand, one may resort to clustering strategies in higher dimensional spaces, as the p neighbors of a given atom are represented by $3p-6$ degrees of freedom – the neighborhood being invariant upon rigid motions. The information gathered while modeling contacts can further be integrated into interface models.

On the topological side, one may favor constructions which remain stable if each atom in a structure *retains* the same neighbors, even though the 3D positions of these neighbors change to some extent. This process is observed in flexible docking cases, and call for the development of methods to encode and compare shapes undergoing tame geometric deformations.

3.5.2. Modeling Macro-molecular Assemblies

In dealing with large assemblies, a number of methodological developments are called for.

[0] Assuming local forces are prominent, which in turn subsumes electrostatic interactions are not prominent.

On the experimental side, of particular interest is the disambiguation of proteomics signals. For example, TAP and mass spectrometry data call for the development of combinatorial algorithms aiming at unraveling pairwise contacts between proteins within an assembly. Likewise, density maps coming from electron microscopy, which are often of intermediate resolution (5-10Å) call the development of noise resilient segmentation and interpretation algorithms. The results produced by such algorithms can further be used to guide the docking of high resolutions crystal structures into maps.

As for modeling, two classes of developments are particularly stimulating. The first one is concerned with the design of algorithms performing reconstruction by data integration, a process reminiscent from non convex optimization. The second one encompasses assessment methods, in order to single out the reconstructions which best comply with the experimental data. For that endeavor, the development of geometric and topological models accommodating uncertainties is particularly important.

3.5.3. Modeling the Flexibility of Macro-molecules

Given a sampling on an energy landscape, a number of fundamental issues actually arise: how does the point cloud describe the topography of the energy landscape (a question reminiscent from Morse theory)? Can one infer the effective number of degrees of freedom of the system over the simulation, and is this number varying? Answers to these questions would be of major interest to refine our understanding of folding and docking, with applications to the prediction of structural properties. It should be noted in passing that such questions are probably related to modeling phase transitions in statistical physics where geometric and topological methods are being used [42].

From an algorithmic standpoint, such questions are reminiscent of *shape learning*. Given a collection of samples on an (unknown) *model*, *learning* consists of guessing the model from the samples – the result of this process may be called the *reconstruction*. In doing so, two types of guarantees are sought: topologically speaking, the reconstruction and the model should (ideally!) be isotopic; geometrically speaking, their Hausdorff distance should be small. Motivated by applications in Computer Aided Geometric Design, surface reconstruction triggered a major activity in the Computational Geometry community over the past ten years [7]. Aside from applications, reconstruction raises a number of deep issues: the study of distance functions to the model and to the samples, and their comparison; the study of Morse-like constructions stemming from distance functions to points; the analysis of topological invariants of the model and the samples, and their comparison.

AIRSEA Project-Team

3. Research Program

3.1. Introduction

Recent events have raised questions regarding the social and economic implications of anthropic alterations of the Earth system, i.e. climate change and the associated risks of increasing extreme events. Ocean and atmosphere, coupled with other components (continent and ice) are the building blocks of the Earth system. A better understanding of the ocean atmosphere system is a key ingredient for improving prediction of such events. Numerical models are essential tools to understand processes, and simulate and forecast events at various space and time scales. Geophysical flows generally have a number of characteristics that make it difficult to model them. This justifies the development of specifically adapted mathematical methods:

- Geophysical flows are strongly non-linear. Therefore, they exhibit interactions between different scales, and unresolved small scales (smaller than mesh size) of the flows have to be **parameterized** in the equations.
- Geophysical fluids are non closed systems. They are open-ended in their scope for including and dynamically coupling different physical processes (e.g., atmosphere, ocean, continental water, etc). **Coupling** algorithms are thus of primary importance to account for potentially significant feedback.
- Numerical models contain parameters which cannot be estimated accurately either because they are difficult to measure or because they represent some poorly known subgrid phenomena. There is thus a need for **dealing with uncertainties**. This is further complicated by the turbulent nature of geophysical fluids.
- The computational cost of geophysical flow simulations is huge, thus requiring the use of **reduced models, multiscale methods** and the design of algorithms ready for **high performance computing** platforms.

Our scientific objectives are divided into four major points. The first objective focuses on developing advanced mathematical methods for both the ocean and atmosphere, and the coupling of these two components. The second objective is to investigate the derivation and use of model reduction to face problems associated with the numerical cost of our applications. The third objective is directed toward the management of uncertainty in numerical simulations. The last objective deals with efficient numerical algorithms for new computing platforms. As mentioned above, the targeted applications cover oceanic and atmospheric modeling and related extreme events using a hierarchy of models of increasing complexity.

3.2. Modeling for oceanic and atmospheric flows

Current numerical oceanic and atmospheric models suffer from a number of well-identified problems. These problems are mainly related to lack of horizontal and vertical resolution, thus requiring the parameterization of unresolved (subgrid scale) processes and control of discretization errors in order to fulfill criteria related to the particular underlying physics of rotating and strongly stratified flows. Oceanic and atmospheric coupled models are increasingly used in a wide range of applications from global to regional scales. Assessment of the reliability of those coupled models is an emerging topic as the spread among the solutions of existing models (e.g., for climate change predictions) has not been reduced with the new generation models when compared to the older ones.

Advanced methods for modeling 3D rotating and stratified flows The continuous increase of computational power and the resulting finer grid resolutions have triggered a recent regain of interest in numerical methods and their relation to physical processes. Going beyond present knowledge requires a better understanding of numerical dispersion/dissipation ranges and their connection to model fine scales. Removing the leading order truncation error of numerical schemes is thus an active topic of research and each mathematical tool has to adapt to the characteristics of three dimensional stratified and rotating flows. Studying the link between discretization errors and subgrid scale parameterizations is also arguably one of the main challenges.

Complexity of the geometry, boundary layers, strong stratification and lack of resolution are the main sources of discretization errors in the numerical simulation of geophysical flows. This emphasizes the importance of the definition of the computational grids (and coordinate systems) both in horizontal and vertical directions, and the necessity of truly multi resolution approaches. At the same time, the role of the small scale dynamics on large scale circulation has to be taken into account. Such parameterizations may be of deterministic as well as stochastic nature and both approaches are taken by the AIRSEA team. The design of numerical schemes consistent with the parameterizations is also arguably one of the main challenges for the coming years. This work is complementary and linked to that on parameters estimation described in 3.4 .

Ocean Atmosphere interactions and formulation of coupled models State-of-the-art climate models (CMs) are complex systems under continuous development. A fundamental aspect of climate modeling is the representation of air-sea interactions. This covers a large range of issues: parameterizations of atmospheric and oceanic boundary layers, estimation of air-sea fluxes, time-space numerical schemes, non conforming grids, coupling algorithms ...Many developments related to these different aspects were performed over the last 10-15 years, but were in general conducted independently of each other.

The aim of our work is to revisit and enrich several aspects of the representation of air-sea interactions in CMs, paying special attention to their overall consistency with appropriate mathematical tools. We intend to work consistently on the physics and numerics. Using the theoretical framework of global-in-time Schwarz methods, our aim is to analyze the mathematical formulation of the parameterizations in a coupling perspective. From this study, we expect improved predictability in coupled models (this aspect will be studied using techniques described in 3.4). Complementary work on space-time nonconformities and acceleration of convergence of Schwarz-like iterative methods (see 7.1.2) are also conducted.

3.3. Model reduction / multiscale algorithms

The high computational cost of the applications is a common and major concern to have in mind when deriving new methodological approaches. This cost increases dramatically with the use of sensitivity analysis or parameter estimation methods, and more generally with methods that require a potentially large number of model integrations.

A dimension reduction, using either stochastic or deterministic methods, is a way to reduce significantly the number of degrees of freedom, and therefore the calculation time, of a numerical model.

Model reduction Reduction methods can be deterministic (proper orthogonal decomposition, other reduced bases) or stochastic (polynomial chaos, Gaussian processes, kriging), and both fields of research are very active. Choosing one method over another strongly depends on the targeted application, which can be as varied as real-time computation, sensitivity analysis (see e.g., section 7.3.1) or optimisation for parameter estimation (see below).

Our goals are multiple, but they share a common need for certified error bounds on the output. Our team has a 4-year history of working on certified reduction methods and has a unique positioning at the interface between deterministic and stochastic approaches. Thus, it seems interesting to conduct a thorough comparison of the two alternatives in the context of sensitivity analysis. Efforts will also be directed toward the development of efficient greedy algorithms for the reduction, and the derivation of goal-oriented sharp error bounds for non linear models and/or non linear outputs of interest. This will be complementary to our work on the deterministic reduction of parametrized viscous Burgers and Shallow Water equations where the objective is to obtain sharp error bounds to provide confidence intervals for the estimation of sensitivity indices.

Reduced models for coupling applications Global and regional high-resolution oceanic models are either coupled to an atmospheric model or forced at the air-sea interface by fluxes computed empirically preventing proper physical feedback between the two media. Thanks to high-resolution observational studies, the existence of air-sea interactions at oceanic mesoscales (i.e., at $\mathcal{O}(1km)$ scales) have been unambiguously shown. Those interactions can be represented in coupled models only if the oceanic and atmospheric models are run on the same high-resolution computational grid, and are absent in a forced mode. Fully coupled models at high-resolution are seldom used because of their prohibitive computational cost. The derivation of a reduced model as an alternative between a forced mode and the use of a full atmospheric model is an open problem.

Multiphysics coupling often requires iterative methods to obtain a mathematically correct numerical solution. To mitigate the cost of the iterations, we will investigate the possibility of using reduced-order models for the iterative process. We will consider different ways of deriving a reduced model: coarsening of the resolution, degradation of the physics and/or numerical schemes, or simplification of the governing equations. At a mathematical level, we will strive to study the well-posedness and the convergence properties when reduced models are used. Indeed, running an atmospheric model at the same resolution as the ocean model is generally too expensive to be manageable, even for moderate resolution applications. To account for important fine-scale interactions in the computation of the air-sea boundary condition, the objective is to derive a simplified boundary layer model that is able to represent important 3D turbulent features in the marine atmospheric boundary layer.

Reduced models for multiscale optimization The field of multigrid methods for optimisation has known a tremendous development over the past few decades. However, it has not been applied to oceanic and atmospheric problems apart from some crude (non-converging) approximations or applications to simplified and low dimensional models. This is mainly due to the high complexity of such models and to the difficulty in handling several grids at the same time. Moreover, due to complex boundaries and physical phenomena, the grid interactions and transfer operators are not trivial to define.

Multigrid solvers (or multigrid preconditioners) are efficient methods for the solution of variational data assimilation problems. We would like to take advantage of these methods to tackle the optimization problem in high dimensional space. High dimensional control space is obtained when dealing with parameter fields estimation, or with control of the full 4D (space time) trajectory. It is important since it enables us to take into account model errors. In that case, multigrid methods can be used to solve the large scales of the problem at a lower cost, this being potentially coupled with a scale decomposition of the variables themselves.

3.4. Dealing with uncertainties

There are many sources of uncertainties in numerical models. They are due to imperfect external forcing, poorly known parameters, missing physics and discretization errors. Studying these uncertainties and their impact on the simulations is a challenge, mostly because of the high dimensionality and non-linear nature of the systems. To deal with these uncertainties we work on three axes of research, which are linked: sensitivity analysis, parameter estimation and risk assessment. They are based on either stochastic or deterministic methods.

Sensitivity analysis Sensitivity analysis (SA), which links uncertainty in the model inputs to uncertainty in the model outputs, is a powerful tool for model design and validation. First, it can be a pre-stage for parameter estimation (see 3.4), allowing for the selection of the more significant parameters. Second, SA permits understanding and quantifying (possibly non-linear) interactions induced by the different processes defining e.g., realistic ocean atmosphere models. Finally SA allows for validation of models, checking that the estimated sensitivities are consistent with what is expected by the theory. On ocean, atmosphere and coupled systems, only first order deterministic SA are performed, neglecting the initialization process (data assimilation). AIRSEA members and collaborators proposed to use second order information to provide consistent sensitivity measures, but so far it has only been applied to simple academic systems. Metamodels are now commonly used, due to the cost induced by each evaluation of complex numerical models: mostly Gaussian processes, whose probabilistic framework allows for the development of specific adaptive designs, and polynomial chaos not only in the context of intrusive Galerkin approaches but also in a black-box approach. Until recently, global SA was based primarily on a set of engineering practices. New mathematical and methodological developments have led to the numerical computation of Sobol' indices, with confidence intervals assessing for both metamodel and estimation errors. Approaches have also been extended to the case of dependent entries, functional inputs and/or output and stochastic numerical codes. Other types of indices and generalizations of Sobol' indices have also been introduced.

Concerning the stochastic approach to SA we plan to work with parameters that show spatio-temporal dependencies and to continue toward more realistic applications where the input space is of huge dimension with highly correlated components. Sensitivity analysis for dependent inputs also introduces new challenges. In our applicative context, it would seem prudent to carefully learn the spatio-temporal dependences before running a global SA. In the deterministic framework we focus on second order approaches where the sought sensitivities are related to the optimality system rather than to the model; i.e., we consider the whole forecasting system (model plus initialization through data assimilation).
All these methods allow for computing sensitivities and more importantly a posteriori error statistics.

Parameter estimation Advanced parameter estimation methods are barely used in ocean, atmosphere and coupled systems, mostly due to a difficulty of deriving adequate response functions, a lack of knowledge of these methods in the ocean-atmosphere community, and also to the huge associated computing costs. In the presence of strong uncertainties on the model but also on parameter values, simulation and inference are closely associated. Filtering for data assimilation and Approximate Bayesian Computation (ABC) are two examples of such association.
Stochastic approach can be compared with the deterministic approach, which allows to determine the sensitivity of the flow to parameters and optimize their values relying on data assimilation. This approach is already shown to be capable of selecting a reduced space of the most influent parameters in the local parameter space and to adapt their values in view of correcting errors committed by the numerical approximation. This approach assumes the use of automatic differentiation of the source code with respect to the model parameters, and optimization of the obtained raw code.

AIRSEA assembles all the required expertise to tackle these difficulties. As mentioned previously, the choice of parameterization schemes and their tuning has a significant impact on the result of model simulations. Our research will focus on parameter estimation for parameterized Partial Differential Equations (PDEs) and also for parameterized Stochastic Differential Equations (SDEs). Deterministic approaches are based on optimal control methods and are local in the parameter space (i.e., the result depends on the starting point of the estimation) but thanks to adjoint methods they can cope with a large number of unknowns that can also vary in space and time. Multiscale optimization techniques as described in 7.2.1 will be one of the tools used. This in turn can be used either to propose a better (and smaller) parameter set or as a criterion for discriminating parameterization schemes. Statistical methods are global in the parameter state but may suffer from the curse of dimensionality. However, the notion of parameter can also be extended to functional parameters. We may consider as parameter a functional entity such as a boundary condition on time, or a probability density function in a stationary regime. For these purposes, non-parametric estimation will also be considered as an alternative.

Risk assessment Risk assessment in the multivariate setting suffers from a lack of consensus on the choice of indicators. Moreover, once the indicators are designed, it still remains to develop estimation procedures, efficient even for high risk levels. Recent developments for the assessment of financial risk have to be considered with caution as methods may differ pertaining to general financial decisions or environmental risk assessment. Modeling and quantifying uncertainties related to extreme events is of central interest in environmental sciences. In relation to our scientific targets, risk assessment is very important in several areas: hydrological extreme events, cyclone intensity, storm surges...Environmental risks most of the time involve several aspects which are often correlated. Moreover, even in the ideal case where the focus is on a single risk source, we have to face the temporal and spatial nature of environmental extreme events. The study of extremes within a spatio-temporal framework remains an emerging field where the development of adapted statistical methods could lead to major progress in terms of geophysical understanding and risk assessment thus coupling data and model information for risk assessment.

Based on the above considerations we aim to answer the following scientific questions: how to measure risk in a multivariate/spatial framework? How to estimate risk in a non stationary context? How to reduce dimension (see 3.3) for a better estimation of spatial risk?

Extreme events are rare, which means there is little data available to make inferences of risk measures. Risk assessment based on observation therefore relies on multivariate extreme value theory. Interacting particle systems for the analysis of rare events is commonly used in the community of computer experiments. An open question is the pertinence of such tools for the evaluation of environmental risk.
Most numerical models are unable to accurately reproduce extreme events. There is therefore a real need to develop efficient assimilation methods for the coupling of numerical models and extreme data.

3.5. High performance computing

Methods for sensitivity analysis, parameter estimation and risk assessment are extremely costly due to the necessary number of model evaluations. This number of simulations require considerable computational resources, depends on the complexity of the application, the number of input variables and desired quality of approximations. To this aim, the AIRSEA team is an intensive user of HPC computing platforms, particularly grid computing platforms. The associated grid deployment has to take into account the scheduling of a huge number of computational requests and the links with data-management between these requests, all of these as automatically as possible. In addition, there is an increasing need to propose efficient numerical algorithms specifically designed for new (or future) computing architectures and this is part of our scientific objectives. According to the computational cost of our applications, the evolution of high performance computing platforms has to be taken into account for several reasons. While our applications are able to exploit space parallelism to its full extent (oceanic and atmospheric models are traditionally based on a spatial domain decomposition method), the spatial discretization step size limits the efficiency of traditional parallel methods. Thus the inherent parallelism is modest, particularly for the case of relative coarse resolution but with very long integration time (e.g., climate modeling). Paths toward new programming paradigms are thus needed. As a step in that direction, we plan to focus our research on parallel in time methods.

New numerical algorithms for high performance computing Parallel in time methods can be classified into three main groups. In the first group, we find methods using parallelism across the method, such as parallel integrators for ordinary differential equations. The second group considers parallelism across the problem. Falling into this category are methods such as waveform relaxation where the space-time system is decomposed into a set of subsystems which can then be solved independently using some form of relaxation techniques or multigrid reduction in time. The third group of methods focuses on parallelism across the steps. One of the best known algorithms in this family is parareal. Other methods combining the strengths of those listed above (e.g., PFASST) are currently under investigation in the community.

Parallel in time methods are iterative methods that may require a large number of iteration before convergence. Our first focus will be on the convergence analysis of parallel in time (Parareal / Schwarz) methods for the equation systems of oceanic and atmospheric models. Our second objective will be on the construction of fast (approximate) integrators for these systems. This part is naturally linked to the model reduction methods of section (7.2.2). Fast approximate integrators are required both in the Schwarz algorithm (where a first guess of the boundary conditions is required) and in the Parareal algorithm (where the fast integrator is used to connect the different time windows). Our main application of these methods will be on climate (i.e., very long time) simulations. Our second application of parallel in time methods will be in the context of optimization methods. In fact, one of the major drawbacks of the optimal control techniques used in 3.4 is a lack of intrinsic parallelism in comparison with ensemble methods. Here, parallel in time methods also offer ways to better efficiency. The mathematical key point is centered on how to efficiently couple two iterative methods (i.e., parallel in time and optimization methods).

AMIB Project-Team

3. Research Program

3.1. RNA and protein structures

At the secondary structure level, we contributed novel generic techniques applicable to dynamic programming and statistical sampling, and applied them to design novel efficient algorithms for probing the conformational space. Another originality of our approach is that we cover a wide range of scales for RNA structure representation. For each scale (atomic, sequence, secondary and tertiary structure...) cutting-edge algorithmic strategies and accurate and efficient tools have been developed or are under development. This offers a new view on the complexity of RNA structure and function that will certainly provide valuable insights for biological studies.

3.1.1. Dynamic programming and complexity

Participants: Yann Ponty, Wei Wang, Antoine Soulé, Juraj Michalik.

*Common activity with J. Waldispühl (McGill) and A. Denise (*Lri*).*

Ever since the seminal work of Zuker and Stiegler, the field of RNA bioinformatics has been characterized by a strong emphasis on the secondary structure. This discrete abstraction of the 3D conformation of RNA has paved the way for a development of quantitative approaches in RNA computational biology, revealing unexpected connections between combinatorics and molecular biology. Using our strong background in enumerative combinatorics, we propose generic and efficient algorithms, both for sampling and counting structures using dynamic programming. These general techniques have been applied to study the sequence-structure relationship [44], the correction of pyrosequencing errors [37], and the efficient detection of multi-stable RNAs (riboswitches) [40], [41].

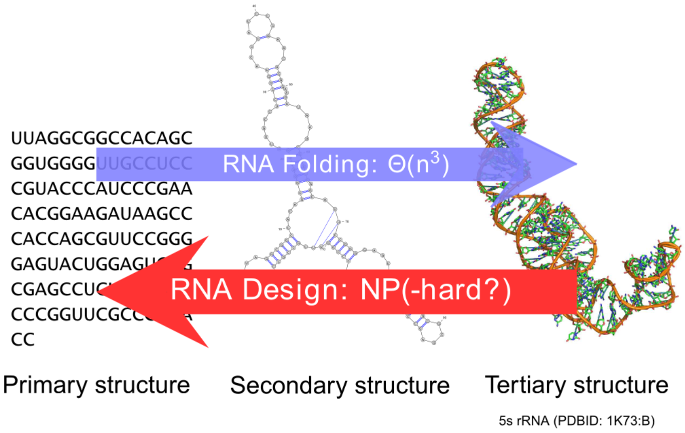


Figure 1. The goal of RNA design, aka RNA inverse folding, is to find a sequence that folds back into a given (secondary) structure.

3.1.2. RNA design.

Participants: Alice Héliou, Yann Ponty.

Joint project with A. Denise (sc Lri), J. Waldispühl (McGill), D. Barash (Univ. Ben-Gurion), and C. Chauve (Simon Fraser University).

It is a natural pursue to build on our understanding of the secondary structure to construct artificial RNAs performing predetermined functions, ultimately targeting therapeutic and synthetic biology applications. Towards this goal, a key element is the design of RNA sequences that fold into a predetermined secondary structure, according to established energy models (inverse-folding problem). Quite surprisingly, and despite two decades of studies of the problem, the computational complexity of the inverse-folding problem is currently unknown.

Within our group, we offer a new methodology, based on weighted random generation [24] and multidimensional Boltzmann sampling, for this problem. Initially lifting the constraint of folding back into the target structure, we explored the random generation of sequences that are compatible with the target, using a probability distribution which favors exponentially sequences of high affinity towards the target. A simple posterior rejection step selects sequences that effectively fold back into the latter, resulting in a *global sampling* pipeline that showed comparable performances to its competitors based on local search [31].

3.1.3. Towards 3D modeling of large molecules

Participants: Yann Ponty, Afaf Saaidi, Mireille Régnier, Amélie Héliou.

*Joint projects with A. Denise (*LRI*), D. Barth (Versailles), J. Cohen (Paris-Sud), B. Sargueil (Paris V) and Jérome Waldispühl (McGill).*

The modeling of large RNA 3D structures, that is predicting the three-dimensional structure of a given RNA sequence, relies on two complementary approaches. The approach by homology is used when the structure of a sequence homologous to the sequence of interest has already been resolved experimentally. The main problem then is to calculate an alignment between the known structure and the sequence. The ab initio approach is required when no homologous structure is known for the sequence of interest (or for some parts of it). We contribute methods inspired by both of these settings directions.

Modeling tasks can also be greatly helped by the availability of experimental data. However, high-resolution techniques such as crystallography or RMN, are notoriously costly in term of time and ressources, leading to the current gap between the amount of available sequences and structural data. As part of a colloboration with B. Sargueil's lab (Faculté de pharmacie, Paris V) funded by the Fondation pour la Recherche medical, we strive to propose a new paradigm for the analysis data produced using a new experimental technique, called SHAPE analysis (Selective 2'-Hydroxyl Acylation analyzed by Primer Extension). This experimental setup produces an accessibility profile associated with the different positions of an RNA, the *shadow* of an RNA. As part of A. Saaidi's PhD, we currently design new algorithmic strategies to infer the secondary structure of RNA from multiple SHAPE experiments performed by experimentalists at Paris V. Those are obtained on mutants, and will be coupled with a fragment-based 3D modeling strategy developed by our partners at McGill.

3.2. Séquences

Participants: Mireille Régnier, Philippe Chassignet, Yann Ponty, Jean-Marc Steyaert, Alice Héliou, Antoine Soulé.

String searching and pattern matching is a classical area in computer science, enhanced by potential applications to genomic sequences. In CPM/SPIRE community, a focus is given to general string algorithms and associated data structures with their theoretical complexity. Our group specialized in a formalization based on languages, weighted by a probabilistic model. Team members have a common expertise in enumeration and random generation of combinatorial sequences or structures, that are *admissible* according to some given constraints. A special attention is paid to the actual computability of formula or the efficiency of structures design, possibly to be reused in external software.

As a whole, motif detection in genomic sequences is a hot subject in computational biology that allows to address some key questions such as chromosome dynamics or annotation. Among specific motifs involved in molecular interactions, one may cite protein-DNA (cis-regulation), protein-protein (docking), RNA-RNA (miRNA, frameshift, circularisation). This area is being renewed by high throughput data and assembly issues. New constraints, such as energy conditions, or sequencing errors and amplification bias that are technology dependent, must be introduced in the models. A collaboration has beenestablished with LOB, at Ecole Polytechnique, who bought a sequencing machine, through the co-advised thesis of Alice Héliou. An other aim is to combine statistical sampling with a fragment based approach for decomposing structures, such as the cycle decomposition used within F. Major's group [33]. In general, in the future, our methods for sampling and sequence data analysis should be extended to take into account such constraints, that are continuously evolving.

3.2.1. Combinatorial Algorithms and motifs

Participants: Mireille Régnier, Philippe Chassignet, Alice Héliou.

Besides applications [39] of analytic combinatorics to computational biology problems, the team addressed general combinatorial problems on words and fundamental issues on languages and data structures.

Motif detection combines an algorithmic search of potential sites and a significance assessment. Assessment significance requires a quantitative criterion such as the p-value.

In the recent years, a general scheme of derivation of analytic formula for the pvalue under different constraints (k-occurrence, first occurrence, overrepresentation in large sequences,...) has been provided. It relies on a representation of continuous sequences of overlapping words, currently named *clumps* or *clusters* in a graph [35]. Recursive equations to compute p-values may be reduced to a traversal of that graph, leading to a linear algorithm. This improves over the space and time complexity of the generating function approach or previous probabilistic weighted automata.

This research area is widened by new problems arising from *de novo* genome assembly or re-assembly.

In [43], it is claimed that half of the genome consists of different types of repeats. One may cite microsatellites, DNA transposons, transposons, long terminal repeats (LTR), long interspersed nuclear elements (LINE), ribosomal DNA, short interspersed nuclear elements (SINE). Therefore, knowledge about the length of repeats is a key issue in several genomic problems, notably assembly or re-sequencing. Preliminary theoretical results are given in [28], and, recently, heuristics have been proposed and implemented [25], [38], [22]. A dual problem is the length of minimal absent words. Minimal absent words are words that do not occur but whose proper factors all occur in the sequence. Their computation is extremly related to finding maximal repeats (repeat that can not be extended on the right nor on the left). The comparison of the sets of minimal absent words provides a fast alternative for measuring approximation in sequence comparison [21], [23].

Recently, it was shown that considering the words which occur in one sequence but do no in another can be used to detect biologically significant events [42]. We have studied the computation of minimal absent words and we have provided new linear implementations [18],[16]. We are now working on a dynamic approach to compute minimal absent words for a sliding window. For a sequence of size n, we expect a complexity of O(n) in time and space, independent of the size of the window. This approach could be use to align a sequence on a larger sequence using minimal absent words for comparison.

According to the current knowledge, cancer develops as a result of the mutational process of the genomic DNA. In addition to point mutations, cancer genomes often accumulate a significant number of chromosomal rearrangements also called structural variants (SVs). Identifying exact positions and types of these variants may lead to track cancer development or select the most appropriate treatment for the patient. Next Generation Sequencing opens the way to the study of structural variants in the genome, as recently described in [20]. This is the subject of an international collaboration with V. Makeev's lab (IOGENE, Moscow), MAGNOME project-team and V. Boeva (Curie Institute). One goal is to combine two detection techniquesbased either on paired-end mapping abnormalities or on variation of the depth of coverage. A second goal is to develop a model of errors, including a statistical model, that takes into account the quality of data from the different sequencing technologies, their volume and their specificities such as the GC-content or the mappability.

3.2.2. Random generation

Participants: Yann Ponty, Juraj Michalik.

Analytical methods may fail when both sequential and structural constraints of sequences are to be modelled or, more generally, when molecular *structures* such as RNA structures have to be handled. The random generation of combinatorial objects is a natural, alternative, framework to assess the significance of observed phenomena. General and efficient techniques have been developed over the last decades to draw objects uniformly at random from an abstract specification. However, in the context of biological sequences and structures, the uniformity assumption becomes unrealistic, and one has to consider non-uniform distributions in order to derive relevant estimates. Typically, context-free grammars can handle certain kinds of long-range interactions such as base pairings in secondary RNA structures.

In 2005, a new paradigm appeared in the *ab initio* secondary structure prediction [26]: instead of formulating the problem as a classic optimization, this new approach uses statistical sampling within the space of solutions. Besides giving better, more robust, results, it allows for a fruitful adaptation of tools and algorithms derived in a purely combinatorial setting. Indeed, in a joint work with A. Denise (LRI), we have done significant and original progress in this area recently [34], [39], including combinatorial models for structures with pseudoknots. Our aim is to combine this paradigm with a fragment based approach for decomposing structures, such as the cycle decomposition used within F. Major's group [33].

3.3. 3D interaction and structure prediction

Participant: Amélie Héliou.

The biological function of macromolecules such as proteins and nucleic acids relies on their dynamic structural nature and their ability to interact with many different partners. This is specially challenging as structure flexibility is key and multi-scale modelling [19], [27] and efficient code are essential [32].

Our project covers various aspects of biological macromolecule structure and interaction modelling and analysis. First protein structure prediction is addressed through combinatorics. The dynamics of these types of structures is also studied using statistical and robotics inspired strategies. Both provide a good starting point to perform 3D interaction modelling, accurate structure and dynamics being essential.

Our group benefits from a good collaboration network, mainly at Stanford University (USA), HKUST (Hong-Kong) and McGill (Canada). The computational expertise in this field of computational structural biology is represented in a few large groups in the world (e.g. Pande lab at Stanford, Baker lab at U.Washington) that have both dry and wet labs. At Inria, our interest for structural biology is shared by the ABS and ORPAILLEUR project-teams. Our activities are however now more centered around protein-nucleic acid interactions, multi-scale analysis, robotics inspired strategies and machine learning than protein-protein interactions, algorithms and geometry. We also shared a common interest for large biomolecules and their dynamics with the NANO-D project team and their adaptative sampling strategy. As a whole, we contribute to the development of geometric and machine learning strategies for macromolecular docking.

Game theory was used by M. Boudard in her PhD thesis, defended in 2015, to predict the 3d structure of RNA. In her PhD thesis, co-advised by J. Cohen (LRI), A. Héliou is extending the approach to predict protein structures.

3.3.1. Robotics-inspired structure and dynamics

Participant: Amélie Héliou.

We recently work one a robotics approach to sample the conformational space of macromolecules like RNAs [1]. The robotics approach allows maintaining the secondary structure of the RNA fixed, as an unfolding is very unlikely and energetically demanding. By this approach we also dramatically reduce the number of degrees of freedom in the molecule. The conformational space becomes possible to be sampled. This reduction does not reduce the quality of the sampling.

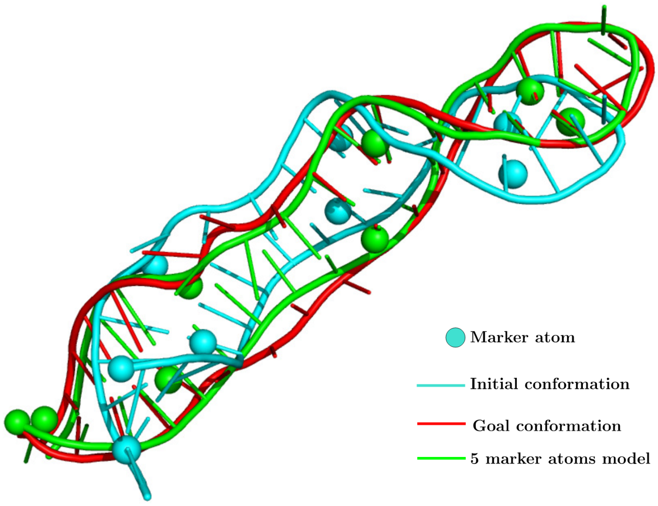


Figure 2. The cyan structure is the initial conformation, the red structure is the goal conformation. The full-atom initial conformation was driven toward the goal conformation using only the position of the goal sphere atoms. The green conformation is the result obtained; spheres perfectly overlap with the goal position and the overall conformation is really close to the goal conformation.

Our current work consists in applying the same approach to a targeted move. The motion is then driven either by the position of a few atoms or the distances between couple of atoms. Theses two aspects are under development and will increase the analysis possibility of experimental data. Our method can drive a RNA conformation toward another conformation of the same RNA given only the position of a few atoms (marker atoms).

For instance double electron-electron resonance (DEER) experimental results are distributions of distances. Probes are attached to the molecules and the distances between to probes is measured and outputted as a distribution. Our method is able to sample an ensemble of all-atom conformations that can explain the distance distribution.

3.3.2. Game theory and protein folding

Participant: Amélie Héliou.

M.Boudard used game theory to sample folded conformations of RNA. We work in apply game theory to sample folded conformations of proteins. This is challenging as a protein is generally less flexible than a RNA and thus accept less conformations.

Our work is first to find an algorithm that can guarantee the convergence to an Nash equilibrium (a state were no player would increase his payoff by playing something different alone) and prove their convergence. At the same time, we are looking for efficient and biologically relevant ways of defining the game settings so that Nash equilibria correspond to folded states. One direction would be to draw a parallel between Nash equilibria and local minima of the kinetic landscape.

ANGE Project-Team

3. Research Program

3.1. Overview

The research activities carried out within the ANGE team strongly couple the development of methodological tools with applications to real–life problems and the transfer of numerical codes. The main purpose is to obtain new models adapted to the physical phenomena at stake, identify the main properties that reflect the physical sense of the models (uniqueness, conservativity, entropy dissipation, ...) and propose effective numerical methods to estimate their solution in complex configurations (multi-dimensional, unstructured meshes, well-balanced, ...).

The difficulties arising in gravity driven flow studies are threefold.

- Models and equations encountered in fluid mechanics (typically the free surface Navier-Stokes equations) are complex to analyze and solve.
- The underlying phenomena often take place over large domains with very heterogeneous length scales (size of the domain, mean depth, wave length,...) and distinct time scales, *e.g.* coastal erosion, propagation of a tsunami,...
- These problems are multi-physics with strong couplings and nonlinearities.

3.2. Modelling and analysis

Hazardous flows are complex physical phenomena that can hardly be represented by shallow water type systems of partial differential equations (PDEs). In this domain, the research program is devoted to the derivation and analysis of reduced complexity models compared to the Navier-Stokes equations, but relaxing the shallow water assumptions. The main purpose is then to obtain models well-adapted to the physical phenomena at stake.

Even if the resulting models do not strictly belong to the family of hyperbolic systems, they exhibit hyperbolic features: the analysis and discretization techniques we intend to develop have connections with those used for hyperbolic conservation laws. It is worth noticing that the need for robust and efficient numerical procedures is reinforced by the smallness of dissipative effects in geophysical models which therefore generate singular solutions and instabilities.

On the one hand, the derivation of the Saint-Venant system from the Navier-Stokes equations is based on two approximations, so-called shallow water assumptions, namely

- the horizontal fluid velocity is well approximated by its mean value along the vertical direction,
- the pressure is hydrostatic or equivalently the vertical acceleration of the fluid can be neglected compared to the gravitational effects.

As a consequence the objective is to get rid of these two assumptions, one after the other, in order to obtain models accurately approximating the incompressible Euler or Navier-Stokes equations.

On the other hand, many applications require the coupling with non-hydrodynamic equations, as in the case of micro-algae production or erosion processes. These new equations comprise non-hyperbolic features and must rely on a special analysis.

3.2.1. Multilayer approach

As for the first shallow water assumption, *multi-layer* systems were proposed describing the flow as a superposition of Saint-Venant type systems [31], [33], [34]. Even if this approach has provided interesting results, layers are considered separate and non-miscible fluids, which imply strong limitation. That is why we proposed a slightly different approach [1], [2] based on Galerkin type decomposition along the vertical axis of all variables and leading, both for the model and its discretization, to more accurate results.

A kinetic representation of our multilayer model allows to derive robust numerical schemes endowed with properties such as: consistency, conservativity, positivity, preservation of equilibria,... It is one of the major achievements of the team but it needs to be analyzed and extended in several directions namely:

- The convergence of the multilayer system towards the hydrostatic Euler system as the number of layers goes to infinity is a critical point. It is not fully satisfactory to have only formal estimates of the convergence and sharp estimates would enable to guess the optimal number of layers.
- The introduction of several source terms due for instance to Coriolis forces or extra terms from changes of coordinates seems necessary. Their inclusion should lead to substantial modifications of the numerical scheme.
- Its hyperbolicity has not yet been proved and conversely the possible loss of hyperbolicity cannot be characterized. Similarly, the hyperbolic feature is essential in the propagation and generation of waves.

3.2.2. Non-hydrostatic models

The hydrostatic assumption consists in neglecting the vertical acceleration of the fluid. It is considered valid for a large class of geophysical flows but is restrictive in various situations where the dispersive effects (like wave propagation) cannot be neglected. For instance, when a wave reaches the coast, bathymetry variations give a vertical acceleration to the fluid that strongly modifies the wave characteristics and especially its height.

When processing an asymptotic expansion (w.r.t. the aspect ratio for shallow water flows) into the Navier-Stokes equations, we obtain at the leading order the Saint-Venant system. Going one step further leads to a vertically averaged version of the Euler/Navier-Stokes equations integrating the non-hydrostatic terms. This model has several advantages:

- it admits an energy balance law (that is not the case for most dispersive models available in the literature),
- it reduces to the Saint-Venant system when the non-hydrostatic pressure term vanishes,
- it consists in a set of conservation laws with source terms,
- it does not contain high order derivatives.

3.2.3. Multi-physics modelling

The coupling of hydrodynamic equations with other equations in order to model interactions between complex systems represents an important part of the team research. More precisely, three multi-physic systems are investigated. More details about the industrial impact of these studies are presented in the following section.

- To estimate the risk for infrastructures in coastal zone or close to a river, the resolution of the shallow water equations with moving bathymetry is necessary. The first step consisted in the study of an equation largely used in engineering science: The Exner equation. The analysis enabled to exhibit drawbacks of the coupled model such as the lack of energy conservation or the strong variations of the solution from small perturbations. A new formulation is proposed to avoid these drawbacks. The new model consists in a coupling between conservation laws and an elliptic equation, like the system Euler/Poisson, suggesting to use well-known strategies for the analysis and the numerical resolution. In addition, the new formulation is derived from classical complex rheology models and allowed physical phenomena such as threshold laws.
- Interaction between flows and floating structures is the challenge at the scale of the shallow water equations. This study needs a better understanding of the energy exchanges between the flow and the structure. The mathematical model of floating structures is very hard to solve numerically due to the non-penetration condition at the interface between the flow and the structure. It leads to infinite potential wave speeds that could not be solved with classical free surface numerical scheme. A relaxation model was derived to overcome this difficulty. It represents the interaction with the floating structure with a free surface model-type.

- If the interactions between hydrodynamics and biology phenomena are known through laboratory experiments, it is more difficult to predict the evolution, especially for the biological quantities, in a real and heterogeneous system. The objective is to model and reproduce the hydrodynamics modifications due to forcing term variations (in time and space). We are typically interested in phenomena such as eutrophication, development of harmful bacteria (cyanobacteria) and upwelling phenomena.

3.3. Numerical analysis

3.3.1. Non-hydrostatic scheme

The main challenge in the study of the non-hydrostatic model is to design a robust and efficient numerical scheme endowed with properties such as: positivity, wet/dry interfaces treatment, consistency. It has to be noticed that even if the non-hydrostatic model looks like an extension of the Saint-Venant system, most of the known techniques used in the hydrostatic case are not efficient as we recover strong difficulties encountered in incompressible fluid mechanics due to the extra pressure term. These difficulties are reinforced by the absence of viscous/dissipative terms.

3.3.2. Space decomposition and adaptive scheme

In the quest for a better balance between accuracy and efficiency, a strategy consists in the adaptation of models. Indeed, the systems of partial differential equations we consider result from a hierarchy of simplifying assumptions. However, some of these hypotheses may turn out to be irrelevant locally. The adaptation of models thus consists in determining areas where a simplified model (*e.g.* shallow water type) is valid and where it is not. In the latter case, we may go back to the “parent” model (*e.g.* Euler) in the corresponding area. This implies to know how to handle the coupling between the aforementioned models from both theoretical and numerical points of view. In particular, the numerical treatment of transmission conditions is a key point. It requires the estimation of characteristic values (Riemann invariant) which have to be determined according to the regime (torrential or fluvial).

3.3.3. Asymptotic-Preserving scheme for source terms

The hydrodynamic models comprise advection and sources terms. The conservation of the balance between the source terms, typically viscosity and friction, has a significant impact since the overall flow is generally a perturbation around one equilibrium. The design of numerical schemes able to preserve such balances is a challenge from both theoretical and industrial points of view.The concept of Asymptotic-Preserving (AP) methods is of great interest in order to overcome these issues.

Another difficulty occurs when a term, typically related to the pressure, becomes very large compared to the order of magnitude of the velocity. At this regime, namely the so-called *low Froude* (shallow water) or *low Mach* (Euler) regimes, the difference between the speed of the potential waves and the physical velocity makes classical numerical schemes not efficient: firstly because of the error of truncation which is inversely proportional to the small parameters, secondly because of the time step governed by the largest speed of the potential wave. AP methods made a breakthrough in the numerical resolution of asymptotic perturbations of partial-differential equations concerning the first point. The second one can be fixed using partially implicit scheme.

3.3.4. Multi-physics models

Coupling problems also arise within the fluid when it contains pollutants, density variations or biological species. For most situations, the interactions are small enough to use a splitting strategy and the classical numerical scheme for each sub-model, whether it be hydrodynamic or non-hydrodynamic.

The sediment transport raises interesting issues from a numerical aspect. This is an example of coupling between the flow and another phenomenon, namely the deformation of the bottom of the basin that can be carried out either by bed load where the sediment has its own velocity or suspended load in which the particles are mostly driven by the flow. This phenomenon involves different time scales and nonlinear retroactions; hence the need for accurate mechanical models and very robust numerical methods. In collaboration with industrial partners (EDF–LNHE), the team already works on the improvement of numerical methods for existing (mostly empirical) models but our aim is also to propose new (quite) simple models that contain important features and satisfy some basic mechanical requirements. The extension of our 3D models to the transport of weighted particles can also be here of great interest.

3.3.5. Optimization

Numerical simulations are a very useful tool for the design of new processes, for instance in renewable energy or water decontamination. The optimization of the process according to a well-defined objective such as the production of energy or the evaluation of a pollutant concentration is the logical upcoming challenge in order to propose competitive solutions in industrial context. First of all, the set of parameters that have a significant impact on the result and on which we can act in practice is identified. Then the optimal parameters can be obtained using the numerical codes produced by the team to estimate the performance for a given set of parameters with an additional loop such as gradient descent or Monte Carlo method. The optimization is used in practice to determine the best profile for turbine pales, the best location for water turbine implantation, in particular for a farm.

ARAMIS Project-Team

3. Research Program

3.1. General aim

The overall aim of our project is to design new computational and mathematical approaches for studying brain structure (based on anatomical and diffusion MRI) and functional connectivity (based on EEG, MEG and intracerebral recordings). The goal is to transform raw unstructured images and signals into formalized, operational models such as geometric models of brain structures, statistical population models, and graph-theoretic models of brain connectivity. This general endeavor is addressed within the three following main objectives.

3.2. Modeling brain structure: from imaging to geometric models

Structural MRI (anatomical or diffusion-weighted) allows studying in vivo the anatomical architecture of the brain. Thanks to the constant advance of these imaging techniques, it is now possible to visualize various anatomical structures and lesions with a high spatial resolution. Computational neuroanatomy aims at building models of the structure of the human brain, based on MRI data. This general endeavor requires addressing the following methodological issues: i) the extraction of geometrical objects (anatomical structures, lesions, white matter tracks...) from anatomical and diffusion-weighted MRI; ii) the design of a coherent mathematical framework to model anatomical shapes and compare them across individuals. Within this context, we pursue the following objectives.

First, we aim to develop new methods to segment anatomical structures and lesions. We are most specifically interested in the hippocampus, a structure playing a crucial role in Alzheimer's disease, and in lesions of vascular origin (such as white matter hyperintensities and microbleeds). We pay particular attention to the robustness of the approaches with respect to normal and pathological anatomical variability and with respect to differences in acquisition protocols, for application to multicenter studies. We dedicate specific efforts to the validation on large populations of coming from patients data acquired in multiple centers.

Then, we develop approaches to estimate templates from populations and compare anatomical shapes, based on a diffeomorphic deformation framework and matching of distributions. These methods allow the estimation of a prototype configuration (called template) that is representative of a collection of anatomical data. The matching of this template to each observation gives a characterization of the anatomical variability within the population, which is used to define statistics. In particular, we aim to design approaches that can integrate multiple objects and modalities, across different spatial scales.

3.3. Modeling dynamical brain networks

Functional imaging techniques (EEG, MEG and fMRI) allow characterizing the statistical interactions between the activities of different brain areas, i.e. functional connectivity. Functional integration of spatially distributed brain regions is a well-known mechanism underlying various cognitive and perceptual tasks. Indeed, mounting evidence suggests that impairment of such mechanisms might be the first step of a chain of events triggering several neurological disorders, such as the abnormal synchronization of epileptic activities. Naturally, neuroimaging studies investigating functional connectivity in the brain have become increasingly prevalent.

Our team develops a framework for the characterization of brain connectivity patterns, based on connectivity descriptors from the theory of complex networks. The description of the connectivity structure of neural networks is able to characterize for instance, the configuration of links associated with rapid/abnormal synchronization and information transfer, wiring costs, resilience to certain types of damage, as well as the balance between local processing and global integration. Furthermore, we propose to extend this framework to study the reconfiguration of networks over time. Indeed, neurophysiological data are often gathered from longitudinal recording sessions of the same subject to study the adaptive reconfiguration of brain connectivity. Finally, connectivity networks are usually extracted from different brain imaging modalities (MEG, EEG, fMRI or DTI) separately. Methods for combining the information carried by these different networks are still missing. We thus propose to combine connectivity patterns extracted from each modality for a more comprehensive characterization of networks.

3.4. Methodologies for large-scale datasets

Until recently, neuroimaging studies were often restricted to series of about 20-30 patients. As a result, such studies had a limited statistical power and could not adequately model the variability of populations. Thanks to wider accessibility of neuroimaging devices and important public and private funding, large-scale studies including several hundreds of patients have emerged in the past years. In the field of Alzheimer’s disease (AD) for instance, one can cite the Alzheimer’s Disease Neuroimaging Initiative (ADNI) including about 800 subjects (patients with AD or mild cognitive impairment (MCI) and healthy controls) or the French cohort MEMENTO including about 2000 subjects with memory complaint. These are most often multicenter studies in which patients are recruited over different centers and images acquired on different scanners. Moreover, cohort studies include a longitudinal component: for each subject, multiple images are acquired at different time points. Finally, such datasets often include multimodal data: neuroimaging, clinical data, cognitive tests and genomics data. These datasets are complex, high-dimensional and often heterogeneous, and thus require the development of new methodologies to be fully exploited.

In this context, our objectives are:

- to develop methodologies to acquire and standardize multicenter neuroimaging data;
- to develop imaging biomarkers based on machine learning and longitudinal models;
- to design multimodal analysis approaches for bridging anatomical models and genomics.

The first two aspects focus on neuroimaging and are tightly linked with the CATI project. The last one builds on our previous expertise in morphometry and machine learning, but aims at opening new research avenues combining imaging and “omics” data. This is developed in strong collaboration with the new biostatistics/bioinformatics platform of the IHU-A-ICM.

ASCLEPIOS Project-Team

3. Research Program

3.1. Introduction

Tremendous progress has been made in the automated analysis of biomedical images during the past two decades [72]. Readers who are neophytes to the field of medical imaging will find an interesting presentation of acquisition techniques of the main medical imaging modalities in [64], [62]. Regarding target applications, a good review of the state of the art can be found in the book *Computer Integrated Surgery* [60], in N. Ayache's article [67] and in recent review articles [68], [72]. The scientific journals *Medical Image Analysis* [55], *Transactions on Medical Imaging* [61], and *Computer Assisted Surgery* [63] are also good reference material. One can have a good vision of the state of the art from the proceedings of the MICCAI'2010 (Medical Image Computing and Computer Assisted Intervention [58], [59]) and ISBI'2010 (Int. Symp. on Biomedical Imaging [57]) conferences.

For instance, for rigid parts of the body like the head, it is now possible to fuse in a completely automated manner images of the same patient taken from different imaging modalities (e.g. anatomical and functional), or to track the evolution of a pathology through the automated registration and comparison of a series of images taken at distant time instants [73], [83]. It is also possible to obtain from a Magnetic Resonance Image (MRI) of the head a reasonable segmentation of skull tissues, white matter, grey matter, and cerebro-spinal fluid [86], or to measure some functional properties of the heart from dynamic sequences of Magnetic Resonance [66], Ultrasound or Nuclear Medicine images [74].

Despite these advances and successes, statistical models of anatomy are still very crude, resulting in poor registration results in deformable regions of the body, or between different subjects. If some algorithms exploit the physical modeling of the image acquisition process, only a few actually model the physical or even the physiological properties of the human body itself. Coupling biomedical image analysis with anatomical and physiological models of the human body could not only provide a better understanding of observed images and signals, but also more efficient tools for detecting anomalies, predicting evolutions, simulating and assessing therapies.

3.2. Medical Image Analysis

The quality of biomedical images tends to improve constantly (better spatial and temporal resolution, better signal to noise ratio). Not only are the images multidimensional (3 spatial coordinates and possibly one temporal dimension), but medical protocols tend to include multisequence (or multiparametric) [0] and multimodal images [0] for each single patient.

[0] Multisequence (or multiparametric) imaging consists in acquiring several images of a given patient with the same imaging modality (e.g. MRI, CT, US, SPECT, etc.) but with varying acquisition parameters. For instance, using MRI, patients followed for multiple sclerosis may undergo every six months a 3D multisequence MR acquisition protocol with different pulse sequences (called T1, T2, PD, Flair, etc.): by varying some parameters of the pulse sequences (e.g Echo Time and Repetition Time), images of the same regions are produced with quite different contrasts depending on the nature and function of the observed structures. In addition, one of the acquisitions (T1) can be combined with the injection of a contrast product (typically Gadolinium) to reveal vessels and some pathologies. Diffusion Tensor Images (DTI) can be acquired to measure the self diffusion of protons in every voxel, allowing the measurement for instance of the direction of white matter fibers in the brain (the same principle can be used to measure the direction of muscular fibers in the heart). Functional MRI of the brain can be acquired by exploiting the so-called Bold Effect (Blood Oxygen Level Dependency): slightly higher blood flow in active regions creates a subtle higher T2* signal which can be detected with sophisticated image processing techniques.

[0] Multimodal acquisition consists in acquiring from the same patient images of different modalities, in order to exploit their complementary nature. For instance, CT and MR may provide information on the anatomy (CT providing contrast between bones and soft tissues while MR within soft tissues of different nature) while SPECT and PET images may provide functional information by measuring a local level of metabolic activity.

Despite remarkable efforts and advances during the past twenty years, the central problems of segmentation and registration have not been solved in the general case. It is our objective in the short term to work on specific versions of these problems, taking into account as much *a priori* information as possible on the underlying anatomy and pathology at hand. It is also our objective to include more knowledge of the physics of image acquisition and observed tissues, as well as of the biological processes involved. Therefore the research activities mentioned in this section will incorporate the advances made in Computational Anatomy and Computational Physiology, as described in sections 3.3 and 3.4 .

We plan to pursue our efforts on the following problems:

- multi-dimensional, multi-sequence and multi-modal image segmentation; and
- image Registration/Fusion.

3.3. Computational Anatomy

The aim of Computational Anatomy (CA) is to model and analyse the biological variability of the human anatomy. Typical applications cover the simulation of average anatomies and normal variations, the discovery of structural differences between healthy and diseased populations, and the detection and classification of pathologies from structural anomalies. [0]

Studying the variability of biological shapes is an old problem (cf. the book "On Shape and Growth" by D'Arcy Thompson [85]). Significant efforts have since been made to develop a theory for statistical shape analysis (one can refer to [71] for a good summary, and to the special issue of Neuroimage [84] for recent developments). Despite all these efforts, there are a number of challenging mathematical issues that remain largely unsolved. A particular issue is the computation of statistics on manifolds that can be of infinite dimension (e.g the group of diffeomorphisms).

There is a classical stratification of the problems into the following 3 levels [80]:

1. construction from medical images of anatomical manifolds of points, curves, surfaces and volumes;
2. assignment of a point to point correspondence between these manifolds using a specified class of transformations (e.g. rigid, affine, diffeomorphism);
3. generation of probability laws of anatomical variation from these correspondences.

We plan to focus our efforts on the following problems:

1. statistics on anatomical manifolds;
2. propagation of variability from anatomical manifolds;
3. linking anatomical variability to image analysis algorithms; and
4. grid-computing strategies to exploit large databases.

3.4. Computational Physiology

The objective of Computational Physiology (CP) is to provide models of the major functions of the human body and numerical methods to simulate them. The main applications are in medicine where CP can for instance be used to better understand the basic processes leading to the appearance of a pathology, to model its probable evolution and to plan, simulate, and monitor its therapy.

[0] The NIH has launched in 2005 the Alzheimer's Disease Neuroimaging Initiative (60 million USD), a multi-center MRI study of 800 patients who will be followed during several years. The aim is to establish new surrogate end-points from the automated analysis of temporal sequences, which is a challenging goal for researchers in Computational Anatomy. The data is to made available to qualified research groups involved or not in the study.

Quite advanced models have already been proposed to study at the molecular, cellular and organ level a number of physiological systems (see for instance [81], [78], [69], [82], [75]). While these models and new ones need to be developed, refined or validated, a grand challenge that we want to address in this project is the automatic adaptation of the model to a given patient by comparing the model with the available biomedical images and signals and possibly also some additional information (e.g. genetic). Building such *patient-specific models* is an ambitious goal, which requires the choice or construction of models with a complexity adapted to the resolution of the accessible measurements and the development of new data assimilation methods coping with massive numbers of measurements and unknowns.

There is a hierarchy of modeling levels for CP models of the human body [70]:

- the first level is mainly geometrical, and addresses the construction of a digital description of the anatomy [65], essentially acquired from medical imagery;
- the second level is physical, involving mainly the biomechanical modeling of various tissues, organs, vessels, muscles and bone structures [76];
- the third level is physiological, involving the modeling of the functions of the major organ systems [77] (e.g. cardiovascular, respiratory, digestive, central or peripheral nervous, muscular, reproductive, hormonal) or some pathological metabolism (e.g. evolution of cancerous or inflammatory lesions, formation of vessel stenoses, etc.); and
- a fourth level is cognitive, modeling the higher functions of the human brain [56].

These different levels of modeling are closely related to each other, and several physiological systems may interact with each other (e.g. the cardiopulmonary interaction [79]). The choice of the resolution at which each level is described is important, and may vary from microscopic to macroscopic, ideally through multiscale descriptions.

Building this complete hierarchy of models is necessary to evolve from a *Visible Human project* (essentially the first level of modeling) to a much more ambitious *Physiological Human project* (see [77], [78]). We will not address all the issues raised by this ambitious project, but instead focus on the topics detailed below. Among them, our objective is to identify some common methods for the resolution of the large inverse problem raised by the coupling of physiological models and medical images for the construction of patient-specific models (e.g. specific variational or sequential methods (EKF), dedicated particle filters). We also plan to develop specific expertise in the extraction of geometrical meshes from medical images for their further use in simulation procedures. Finally, computational models can be used for specific image analysis problems studied in section 3.2 (e.g. segmentation, registration, tracking). Application domains include

1. surgery simulation;
2. cardiac Imaging;
3. brain tumors, neo-angiogenesis, wound healing processes, ovocyte regulation, etc.

3.5. Clinical Validation

If the objective of many of the research activities of the project is the discovery of original methods and algorithms with a proof of its feasibility in a limited number of representative cases (i.e. proofs of concept) and publications in high quality scientific journals, we believe that it is important that a reasonable number of studies include a much more significant validation effort. As the BioMedical Image Analysis discipline becomes more mature, validation is necessary for the transformation of new ideas into clinical tools and/or industrial products. It also helps to get access to larger databases of images and signals, which in turn help to stimulate new ideas and concepts.

ATHENA Project-Team

3. Research Program

3.1. Computational diffusion MRI

Diffusion MRI (dMRI) provides a non-invasive way of estimating in-vivo CNS fiber structures using the average random thermal movement (diffusion) of water molecules as a probe. It's a recent field of research with a history of roughly three decades. It was introduced in the mid 80's by Le Bihan et al [90], Merboldt et al [94] and Taylor et al [103]. As of today, it is the unique non-invasive technique capable of describing the neural connectivity in vivo by quantifying the anisotropic diffusion of water molecules in biological tissues.

3.1.1. Diffusion Tensor Imaging & High Angular Resolution Diffusion Imaging

In dMRI, the acquisition and reconstruction of the diffusion signal allows for the reconstruction of the water molecules displacement probability, known as the Ensemble Average Propagator (EAP) [102], [72]. Historically, the first model in dMRI is the 2nd order diffusion tensor (DTI) [70], [69] which assumes the EAP to be Gaussian centered at the origin. DTI has now proved to be extremely useful to study the normal and pathological human brain [91], [80]. It has led to many applications in clinical diagnosis of neurological diseases and disorder, neurosciences applications in assessing connectivity of different brain regions, and more recently, therapeutic applications, primarily in neurosurgical planning. An important and very successful application of diffusion MRI has been brain ischemia, following the discovery that water diffusion drops immediately after the onset of an ischemic event, when brain cells undergo swelling through cytotoxic edema.

The increasing clinical importance of diffusion imaging has drived our interest to develop new processing tools for Diffusion Tensor MRI. Because of the complexity of the data, this imaging modality raises a large amount of mathematical and computational challenges. We have therefore developed original and efficient algorithms relying on Riemannian geometry, differential geometry, partial differential equations and front propagation techniques to correctly and efficiently estimate, regularize, segment and process Diffusion Tensor MRI (DT-MRI) (see [93] and [92]).

In DTI, the Gaussian assumption over-simplifies the diffusion of water molecules. While it is adequate for voxels in which there is only a single fiber orientation (or none), it breaks for voxels in which there are more complex internal structures and limitates the ability of the DTI to describe complex, singular and intricate fiber configurations (U-shape, kissing or crossing fibers). To overcome this limitation, so-called Diffusion Spectrum Imaging (DSI) [107] and High Angular Resolution Diffusion Imaging (HARDI) methods such as Q-ball imaging [105] and other multi-tensors and compartment models [100], [101], [63], [62], [98] were developed to resolve the orientationnality of more complicated fiber bundle configurations.

Q-Ball imaging (QBI) has been proven very successful in resolving multiple intravoxel fiber orientations in MR images, thanks tO its ability to reconstruct the Orientation Distribution Function (ODF, the probability of diffusion in a given direction). These tools play a central role in our work related to the development of a robust and linear spherical harmonic estimation of the HARDI signal and to our development of a regularized, fast and robust analytical QBI solution that outperforms the state-of-the-art ODF numerical technique developed by Tuch. Those contributions are fundamental and have already started to impact on the Diffusion MRI, HARDI and Q-Ball Imaging community [79]. They are at the core of our probabilistic and deterministic tractography algorithms devised to best exploit the full distribution of the fiber ODF (see [76], [5] and [77],[6]).

3.1.2. Beyond DTI with high order tensors

High Order Tensors (HOT) models to estimate the diffusion function while overcoming the shortcomings of the 2nd order tensor model have also been recently proposed such as the Generalized Diffusion Tensor Imaging (G-DTI) model developed by Ozarslan et al [109], [110] or 4th order Tensor Model [68]. For more details, we refer the reader to our articles in [81], [100] where we review HOT models and to our articles in [92], co-authored with some of our close collaborators, where we review recent mathematical models and computational methods for the processing of Diffusion Magnetic Resonance Images, including state-of-the-art reconstruction of diffusion models, cerebral white matter connectivity analysis, and segmentation techniques. Recently, we started to work on Diffusion Kurtosis Imaging (DKI), of great interest for the company OLEA MEDICAL. Indeed, DKI is fast gaining popularity in the domain for characterizing the diffusion propagator or EAP by its deviation from Gaussianity. Hence it is an important tool in the clinic for characterizing the white-matter's integrity with biomarkers derived from the 3D 4th order kurtosis tensor (KT) [84].

All these powerful techniques are of utmost importance to acquire a better understanding of the CNS mechanisms and have helped to efficiently tackle and solve a number of important and challenging problems [62], [63]. They have also opened up a landscape of extremely exciting research fields for medicine and neuroscience. Hence, due to the complexity of the CNS data and as the magnetic field strength of scanners increase, as the strength and speed of gradients increase and as new acquisition techniques appear [4], these imaging modalities raise a large amount of mathematical and computational challenges at the core of the research we develop at ATHENA [83], [100].

3.1.3. Improving dMRI acquisitions

One of the most important challenges in diffusion imaging is to improve acquisition schemes and analyse approaches to optimally acquire and accurately represent diffusion profiles in a clinically feasible scanning time. Indeed, a very important and open problem in Diffusion MRI is related to the fact that HARDI scans generally require many times more diffusion gradient than traditional diffusion MRI scan times. This comes at the price of longer scans, which can be problematic for children and people with certain diseases. Patients are usually unable to tolerate long scans and excessive motion of the patient during the acquisition process can force a scan to be aborted or produce useless diffusion MRI images. Recently, we have developed novel methods for the acquisition and the processing of diffusion magnetic resonance images, to efficiently provide, with just few measurements, new insights into the structure and anatomy of the brain white matter in vivo.

First, we contributed developing real-time reconstruction algorithm based on the Kalman filter [75]. Then, and more recently, we started to explore the utility of Compressive Sensing methods to enable faster acquisition of dMRI data by reducing the number of measurements, while maintaining a high quality for the results. Compressed Sensing (CS) is a recent technique which has been proved to accurately reconstruct sparse signals from undersampled measurements acquired below the Shannon-Nyquist rate [95].

We have contributed to the reconstruction of the diffusion signal and its important features as the orientation distribution function and the ensemble average propagator, with a special focus on clinical setting in particular for single and multiple Q-shell experiments [95], [73], [74]. Compressive sensing as well as the parametric reconstruction of the diffusion signal in a continuous basis of functions such as the Spherical Polar Fourier basis, have been proved through our recent contributions to be very useful for deriving simple and analytical closed formulae for many important dMRI features, which can be estimated via a reduced number of measurements [95], [73], [74].

We have also contributed to design optimal acquisition schemes for single and multiple q-shell experiments. In particular, the method proposed in [4] helps generate sampling schemes with optimal angular coverage for multi-shell acquisitions. The cost function we proposed is an extension of the electrostatic repulsion to multi-shell and can be used to create acquisition schemes with incremental angular distribution, compatible with prematurely stopped scans. Compared to more commonly used radial sampling, our method improves the angular resolution, as well as fiber crossing discrimination. The optimal sampling schemes, freely available for download [0], have been selected for use in the HCP (Human Connectome Project) [0].

We think that such kind of contributions open new perspectives for dMRI applications including, for example, tractography where the improved characterization of the fiber orientations is likely to greatly and quickly help tracking through regions with and/or without crossing fibers [82]

[0] http://www.emmanuelcaruyer.com/

[0] http://humanconnectome.org/documentation/Q1/imaging-protocols.html

3.1.4. dMRI modelling, tissue microstructures features recovery & applications

The dMRI signal is highly complex, hence, the mathematical tools required for processing it have to be commensurate in their complexity. Overall, these last twenty years have seen an explosion of intensive scientific research which has vastly improved and literally changed the face of dMRI. In terms of dMRI models, two trends are clearly visible today: the parametric approaches which attempt to build models of the tissue to explain the signal based on model-parameters such as CHARMED [64], AxCaliber [65] and NODDI [108] to cite but a few, and the non-parametric approaches, which attempt to describe the signal in useful but generic functional bases such as the Spherical Polar Fourier (SPF) basis [67], [66], the Solid Harmonic (SoH) basis [78], the Simple Harmonic Oscillator based Reconstruction and Estimation (SHORE) basis [96] and more recent Mean Apparent Propagator or MAP-MRI basis [97].

However, although great improvements have been made in the last twenty years, major improvements are still required primarily to optimally acquire dMRI data, better understand the biophysics of the signal formation, recover invariant and intrinsic microstructure features, identify bio-physically important bio-markers and improve tractography. For short, there is still considerable room for improvement to take dMRI from the benchside to the bedside.

Therefore, there is still considerable room for improvement when it comes to the concepts and tools able to efficiently acquire, process and analyze the complex structure of dMRI data. Develop ground-breaking tools and models for dMRI is one of the major objectives we would like to achieve in order to lead to a decisive advance and breakthrough in this field.

Then, we propose to investigate the feasibility of using our new models and methods to measure extremely important biological tissue microstructure quantities such as axonal radius and density in white matter. These parameters could indeed provide new insight to better understand the brain's architecture and more importantly could also provide new imaging bio-markers to characterize certain neurodegenerative diseases. This challenging scientific problem, when solved, will lead to direct measurements of important microstructural features that will be integrated in our analysis to provide much greater insight into disease mechanisms, recovery and development. These new microstructural parameters will open the road to go far beyond the limitations of the more simple bio-markers derived from DTI that are clinically used to this date – such as MD and FA which are known to be extremely sensitive to confounding factors such as partial volume and axonal dispersion, non-specific and not able to capture any subtle effects that might be early indicators of diseases [7].

3.1.5. Towards microstructural based tractography

In order to go far beyond traditional fiber-tracking techniques, we believe that first order information, i.e. fiber orientations, has to be superseeded by second and third order information, such as microstructure details, to improve tractography. However, many of these higher order information methods are relatively new or unexplored and tractography algorithms based on these high order based methods have to be conceived and designed. In this aim, we propose to work with multiple-shells to reconstruct the Ensemble Average Propagator (EAP), which represents the whole 3D diffusion process and use the possibility it offers to deduce valuable insights on the microstructural properties of the white matter. Indeed, from a reconstructed EAP one can compute the angular features of the diffusion in an diffusion Orientation Distribution Function (ODF), providing insight in axon orientation, calculate properties of the entire diffusion in a voxel such as the Mean Squared Diffusivity (MSD) and Return-To-Origin Probability (RTOP), or come forth with bio-markers detailing diffusion along a particular white matter bundle direction such as the Return-to-Axis or Return-to-Plane Probability (RTAP or RTPP). This opens the way to a ground-breaking computational and unified framework for tractography based on EAP and microstructure features [8]. Using additional a priori anatomical [11] and/or functional information, we could also constrain the tractography algorithm to start and terminate the streamlines only at valid processing areas of the brain.

This development of a computational and unified framework for tractography, based on EAP, microstructure and a priori anatomical and/or functional features, will open new perspectives in tractography, paving the way to a new generation of realistic and biologically plausible algorithms able to deal with intricate configurations of white matter fibers and to provide an exquisite and intrinsic brain connectivity quantification.

3.2. MEG and EEG

Electroencephalography (EEG) and Magnetoencephalography (MEG) are two non-invasive techniques for measuring (part of) the electrical activity of the brain. While EEG is an old technique (Hans Berger, a German neuropsychiatrist, measured the first human EEG in 1929), MEG is a rather new one: the first measurements of the magnetic field generated by the electrophysiological activity of the brain were made in 1968 at MIT by D. Cohen. Nowadays, EEG is relatively inexpensive and is routinely used to detect and qualify neural activities (epilepsy detection and characterisation, neural disorder qualification, BCI, ...). MEG is, comparatively, much more expensive as SQUIDS only operate under very challenging conditions (at liquid helium temperature) and as a specially shielded room must be used to separate the signal of interest from the ambient noise. However, as it reveals a complementary vision to that of EEG and as it is less sensitive to the head structure, it also bears great hopes and an increasing number of MEG machines are being installed throughout the world. Inria and ODYSSÉE/ATHENA have participated in the acquisition of one such machine installed in the hospital "La Timone" in Marseille.

MEG and EEG can be measured simultaneously (M/EEG) and reveal complementary properties of the electrical fields. The two techniques have temporal resolutions of about the millisecond, which is the typical granularity of the measurable electrical phenomena that arise within the brain. This high temporal resolution makes MEG and EEG attractive for the functional study of the brain. The spatial resolution, on the contrary, is somewhat poor as only a few hundred data points can be acquired simultaneously (about 300-400 for MEG and up to 256 for EEG). MEG and EEG are somewhat complementary with fMRI and SPECT in that those provide a very good spatial resolution but a rather poor temporal resolution (of the order of a second for fMRI and a minute for SPECT). Also, contrarily to fMRI, which "only" measures an haemodynamic response linked to the metabolic demand, MEG and EEG measure a direct consequence of the electrical activity of the brain: it is acknowledged that the signals measured by MEG and EEG correspond to the variations of the post-synaptic potentials of the pyramidal cells in the cortex. Pyramidal neurons compose approximately 80% of the neurons of the cortex, and it requires at least about 50,000 active such neurons to generate some measurable signal.

While the few hundred temporal curves obtained using M/EEG have a clear clinical interest, they only provide partial information on the localisation of the sources of the activity (as the measurements are made on or outside of the head). Thus the practical use of M/EEG data raises various problems that are at the core of the ATHENA research in this topic:

- First, as acquisition is continuous and is run at a rate up to 1kHz, the amount of data generated by each experiment is huge. Data selection and reduction (finding relevant time blocks or frequency bands) and pre-processing (removing artifacts, enhancing the signal to noise ratio, ...) are largely done manually at present. Making a better and more systematic use of the measurements is an important step to optimally exploit the M/EEG data [3].
- With a proper model of the head and of the sources of brain electromagnetic activity, it is possible to simulate the electrical propagation and reconstruct sources that can explain the measured signal. Proposing better models [89], [10] and means to calibrate them [106] so as to have better reconstructions are other important aims of our work.
- Finally, we wish to exploit the temporal resolution of M/EEG and to apply the various methods we have developed to better understand some aspects of the brain functioning, and/or to extract more subtle information out of the measurements. This is of interest not only as a cognitive goal, but it also serves the purpose of validating our algorithms and can lead to the use of such methods in the field of Brain Computer Interfaces. To be able to conduct such kind of experiments, an EEG lab has been set up at ATHENA.

BEAGLE Project-Team

3. Research Program

3.1. Introduction

As stated above, the research topics of the BEAGLE Team are centered on the modelisation and simulation of cellular processes. More specifically, we focus on two specific processes that govern cell dynamics and behavior: Evolution and Biophysics. This leads to two main topics: computational cell biology and models for genome evolution.

3.2. Computational Cell Biology

BEAGLE contributes computational models and simulations to the study of cell signaling in prokaryotic and eukaryotic cells, with a special focus on the dynamics of cell signaling both in time and in space. Importantly, our objective here is not so much to produce innovative computer methodologies, but rather to improve our knowledge of the field of cell biology by means of computer methodologies.

This objective is not accessible without a thorough immersion in experimental cell biology. Hence, one specificity of BEAGLE is to be closely associated inside each research project with experimental biology groups. For instance, all the current PhD students implicated in the research projects below have strong interactions with experimenters, most of them conducting experiments themselves in our collaborators' labs. In such a case, the supervision of their PhD is systematically shared between an experimentalist and a theoretician (modeler/computer scientist).

Standard modeling works in cell biochemistry are usually based on mean-field equations, most often referred to as "laws of mass-action". Yet, the derivation of these laws is based on strict assumptions. In particular, the reaction medium must be dilute, perfectly-mixed, three-dimensional and spatially homogeneous and the resulting kinetics are purely deterministic. Many of these assumptions are obviously violated in cells. As already stressed out before, the external membrane or the interior of eukaryotic as well as prokaryotic cells evidence spatial organization at several length scales, so that they must be considered as non-homogeneous media. Moreover, in many case, the small number of molecule copies present in the cell violates the condition for perfect mixing, and more generally, the "law of large numbers" supporting mean-field equations.

When the laws-of-mass-action are invalidated, individual-based models (IBM) appear as the best modeling alternative to evaluate the impact of these specific cellular conditions on the spatial and temporal dynamics of the signaling networks. We develop Individual-Based Models to evaluate the fundamental impact of non-homogeneous space conditions on biochemical diffusion and reaction. More specifically, we focus on the effects of two major sources of non-homogeneity within cells: macromolecular crowding and non-homogeneous diffusion. Macromolecular crowding provides obstacles to the diffusive movement of the signaling molecules, which may in turn have a strong impact on biochemical reactions [45]. In this perspective, we use IBM to renew the interpretation of the experimental literature on this aspect, in particular in the light of the available evidence for anomalous subdiffusion in living cells. Another pertinent source of non-homogeneity is the presence of lipid rafts and/or caveolae in eukaryotic cell membranes that locally alter diffusion. We showed several properties of these diffusion gradients on cells membranes. In addition, combining IBMs and cell biology experiments, we investigate the spatial organization of membrane receptors in plasmic membranes and the impact of these spatial features on the initiation of the signaling networks [49]. More recently, we started to develop IBMs to propose experimentally-verifiable tests able to distinguish between hindered diffusion due to obstacles (macromolecular crowding) and non-homogeneous diffusion (lipid rafts) in experimental data.

The last aspect we tackle concerns the stochasticity of gene expression. Indeed, the stochastic nature of gene expression at the single cell level is now a well established fact [55]. Most modeling works try to explain this stochasticity through the small number of copies of the implicated molecules (transcription factors, in particular). In collaboration with the experimental cell biology group led by Olivier Gandrillon at the Centre de Génétique et de Physiologie Moléculaire et Cellulaire (CGPhyMC, UMR CNRS 5534), Lyon, we study how stochastic gene expression in eukaryotic cells is linked to the physical properties of the cellular medium (e.g., nature of diffusion in the nucleoplasm, promoter accessibility to various molecules, crowding). We have already developed a computer model whose analysis suggests that factors such as chromatin remodeling dynamics have to be accounted for [51]. Other works introduce spatial dimensions in the model, in particular to estimate the role of space in complex (protein+ DNA) formation. Such models should yield useful insights into the sources of stochasticity that are currently not explained by obvious causes (e.g. small copy numbers).

3.3. Models of genome evolution

Classical artificial evolution frameworks lack the basic structure of biological genome (i.e. a double-strand sequence supporting variable size genes separated by variable size intergenic sequences). Yet, if one wants to study how a mutation-selection process is likely (or not) to result in particular biological structures, it is mandatory that the effect of mutation modifies this structure in a realistic way. We have developed an artificial chemistry based on a mathematical formulation of proteins and of the phenotypic traits. In our framework, the digital genome has a structure similar to prokaryotic genomes and a non-trivial genotype-phenotype map. It is a double-stranded genome on which genes are identified using promoter-terminator- like and start-stop-like signal sequences. Each gene is transcribed and translated into an elementary mathematical element (a "protein") and these elements - whatever their number - are combined to compute the phenotype of the organism. The Aevol (Artificial EVOLution) model is based on this framework and is thus able to represent genomes with variable length, gene number and order, and with a variable amount of non-coding sequences (for a complete description of the model, see [63]).

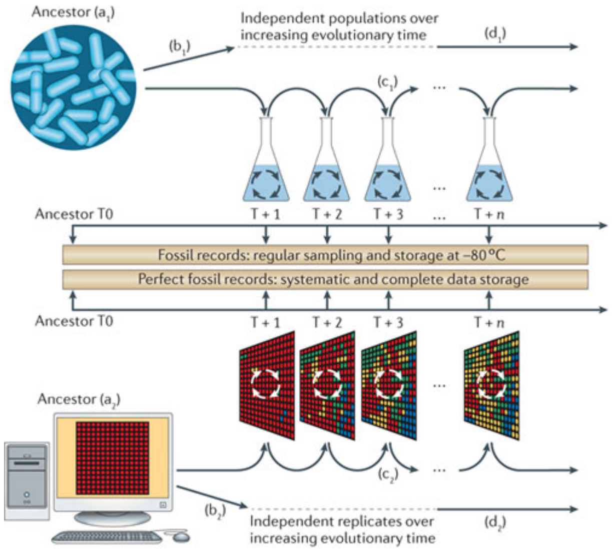

Ancestor (a_1)
(b_1)
Independent populations over increasing evolutionary time
(d_1)
(c_1)
...
Ancestor T0
T + 1
T + 2
T + 3
...
T + n
Fossil records: regular sampling and storage at –80 °C
Perfect fossil records: systematic and complete data storage
Ancestor T0
T + 1
T + 2
T + 3
T + n
Ancestor (a_2)
(c_2)
(b_2)
Independent replicates over increasing evolutionary time
(d_2)

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Figure 1. Parallel between experimental evolution and artificial evolution

As a consequence, this model can be used to study how evolutionary pressures like the ones for robustness or evolvability can shape genome structure [64], [61], [62], [71]. Indeed, using this model, we have shown that genome compactness is strongly influenced by indirect selective pressures for robustness and evolvability. By genome compactness, we mean several structural features of genome structure, like gene number, amount of non functional DNA, presence or absence of overlapping genes, presence or absence of operons [64], [61], [72]. More precisely, we have shown that the genome evolves towards a compact structure if the rate of spontaneous mutations and rearrangements is high. As far as gene number is concerned, this effect was known as an error-threshold effect [54]. However, the effect we observed on the amount of non functional DNA was unexpected. We have shown that it can only be understood if rearrangements are taken into account: by promoting large duplications or deletions, non functional DNA can be mutagenic for the genes it surrounds.

We have extended this framework to include genetic regulation (R-Aevol variant of the model). We are now able to study how these pressures also shape the structure and size of the genetic network in our virtual organisms [47], [46], [48],[29]. Using R-Aevol we have been able to show that (i) the model qualitatively reproduces known scaling properties in the gene content of prokaryotic genomes and that (ii) these laws are not due to differences in lifestyles but to differences in the spontaneous rates of mutations and rearrangements [46]. Our approach consists in addressing unsolved questions on Darwinian evolution by designing controlled and repeated evolutionary experiments, either to test the various evolutionary scenarios found in the literature or to propose new ones. Our experience is that “thought experiments” are often misleading: because evolution is a complex process involving long-term and indirect effects (like the indirect selection of robustness and evolvability), it is hard to correctly predict the effect of a factor by mere thinking. The type of models we develop are particularly well suited to provide control experiments or test of null hypotheses for specific evolutionary scenarios. We often find that the scenarios commonly found in the literature may not be necessary, after all, to explain the evolutionary origin of a specific biological feature. No selective cost to genome size was needed to explain the evolution of genome compactness [64], and no difference in lifestyles and environment was needed to explain the complexity of the gene regulatory network [46]. When we unravel such phenomena in the individual-based simulations, we try to build “simpler” mathematical models (using for instance population genetics-like frameworks) to determine the minimal set of ingredients required to produce the effect. Both approaches are complementary: the individual-based model is a more natural tool to interact with biologists, while the mathematical models contain fewer parameters and fewer ad-hoc hypotheses about the cellular chemistry.

At this time, simulating the evolution of large genomes during hundreds of thousands of generation with the Aevol software can take several weeks or even months. It is worse with R-aevol, where we not only simulate mutations and selection at the evolutionary timescale, but also simulate the lifetime of the individuals, allowing them to respond to environmental signals. Previous efforts to parallelize and distribute Aevol had yielded limited results due to the lack of dedicated staff on these problems. Since September 2014, we have been improving the performance of (R-)Aevol. Thanks to the ADT Aevol, one and a half full time engineers work on improving Aevol and especially to parallelize it. Moreover, we are working to formalize the numerical computation problems with (R-)Aevol to use state-of-the-art optimization techniques from the HPC community. It ranges from dense and sparse matrix multiplication and their optimizations (such as Tridiagonal matrix algorithm) to using new generation accelerator (Intel Xeon Phi and NVidia GPU). However, our goal is not to become a HPC nor a numerical computation team but to work with well-established teams in these fields, such as through the Joint Laboratory for Extreme-Scale Computing, but also with Inria teams in these fields (e.g. ROMA, Avalon, Corse, Storm, DataMove). By doing so, (R-)Aevol simulations will be faster, allowing us to study more parameters in a shorter time. Furthermore, we will also be able to simulate more realistic population sizes, that currently do not fit into the memory of a single computer.

In 2016 we have improved both the quality and the performance of the code. We are currently investigating advance usage of OpenMP to be able to offload part of our execution to accelerator. In particular, we are currently evaluating the performance of the OpenMP version of Aevol on Xeon Phi KNL and on NVidia GPU. In collaboration with the Avalon team and with the help of a shared internship (Mehdi Ghesh), we have build a benchmark for ordinary differential equation (ODE). This benchmark is based on a representative sample of the ODEs (formalizing the genetic network) found within the R-Aevol model. Thanks to this benchmark, we can compare different ODE solvers and methods. Furthermore, researchers working on ODE solvers and methods could use it to evaluate the quality of their approach. We are now working with Avalon team on an algorithm that will automatically choose at runtime the best fitting solver and method (from a performance and a quality of results point of view). Through this collaboration, we have also extended the execo experimental engine [59] to support Aevol and R-Aevol. By doing so, we have now a complete automatic workflow to conduct large scale campaign experiments with thousands of different parameters of our model and use the resources of distributed platform (Grid'5000, CC-IN2P3 and a dedicated cluster).

Since 2014, we are also working on a second model of genome evolution.This new model, developed by the team within the Evoevo european Project, encompasses not only the gene regulation network (as R-aevol does) but also the metabolic level [8]. It allows us to have a real notion of resources and thus to have more complex ecological interactions between the individuals. To speed up computations, the genomic level is simplified compared to aevol, as a chromosome is modelled as a sequence of genes and regulatory elements and not as a sequence of nucleotides. Both models are thus complementary.

Little has been achieved concerning the validation of these models, and the relevance of the observed evolutionary tendencies for living organisms. Some comparisons have been made between Avida and experimental evolution [65], [58], but the comparison with what happened in a long timescale to life on earth is still missing. It is partly because the reconstruction of ancient genomes from the similarities and differences between extant ones is a difficult computational problem which still misses good solutions for every type of mutations, in particular the ones concerning changes in the genome structure.

There exist good phylogenic models of punctual mutations on sequences [56], which enable the reconstruction of small parts of ancestral sequences, individual genes for example [66]. But models of whole genome evolution, taking into account large scale events like duplications, insertions, deletions, lateral transfer, rearrangements are just being developped [74], [52]. Integrative phylogenetic models, considering both nucleotide subsitutions and genome architectures, like Aevol does, are still missing.

Partial models lead to evolutionary hypotheses on the birth and death of genes [53], on the rearrangements due to duplications [44], [73], on the reasons of variation of genome size [60], [67]. Most of these hypotheses are difficult to test due to the difficulty of *in vivo* evolutionary experiments.

To this aim, we develop evolutionary models to reconstruct the history of organisms from the comparison of their genome, at every scale, from nucleotide substitutions to genome organisation rearrangements. These models include large-scale duplications as well as loss of DNA material, and lateral gene transfers from distant species. In particular we have developed models of evolution by rearrangements [68], methods for reconstructing the organization of ancestral genomes [69], [50], [70], or for detecting lateral gene transfer events [43], [10]. It is complementary with the Aevol development because both the model of artificial evolution and the phylogenetic models we develop emphasize on the architecture of genomes. So we are in a good position to compare artificial and biological data on this point.

We improve the phylogenetic models to reconstruct ancestral genomes, jointly seen as gene contents, orders, organizations, sequences. It requires integrative models of genome evolution, which is desirable not only because they will provide a unifying view on molecular evolution, but also because they will shed light onto the relations between different kinds of mutations, and enable the comparison with artificial experiments from models like Aevol.

Based on this experience, the BEAGLE team contributes individual-based and mathematical models of genome evolution, in silico experiments as well as historical reconstruction on real genomes, to shed light on the evolutionary origin of the complex properties of cells.

BIGS Project-Team

3. Research Program

3.1. Introduction

We give here the main lines of our research that belongs to the domains of probability and statistics. For a better understanding, we made the choice to structure them in four items. Although this choice was not arbitrary, the outlines between these items are sometimes fuzzy because each of them deals with modeling and inference and they are all interconnected.

3.2. Stochastic modeling

Our aim is to propose relevant stochastic frameworks for the modeling and the understanding of biological systems. The stochastic processes are particularly suitable for this purpose. Among them, Markov chains give a first framework for the modeling of population of cells [105], [69]. Piecewise deterministic processes are non diffusion processes also frequently used in the biological context [53], [68], [61], [56]. Among Markov model, we also developed strong expertise about processes derived from Brownian motion and Stochastic Differential Equations [94], [67], [96]. For instance, knowledge about Brownian or random walk excursions [104], [93] helps to analyse genetic sequences and to develop inference about it. However, nature provides us with many examples of systems such that the observed signal has a given Hölder regularity, which does not correspond to the one we might expect from a system driven by ordinary Brownian motion. This situation is commonly handled by noisy equations driven by Gaussian processes such as fractional Brownian motion or (in higher dimensions of the parameter) fractional fields. The basic aspects of these differential equations are now well understood, mainly thanks to the so-called *rough paths* tools [80], but also invoking the Russo-Vallois integration techniques [95]. The specific issue of Volterra equations driven by fBm, which is central for the subdiffusion within proteins problem, is addressed in [54]. Many generalizations (Gaussian or not) of this model have been recently proposed, see for instance [44] for some Gaussian locally self-similar fields, [73] for some non-Gaussian models, [47] for anisotropic models. Our team has thus contributed [52], [74], [73], [75], [87] and still contributes [46], [48], [47], [76], [64] to this theoretical study: Hölder continuity, fractal dimensions, existence and uniqueness results for differential equations, study of the laws to quote a few examples. On the other hand, because of the observation of longitudinal data for each subject in medicine, we have to care about the random effect due to the subject and to choose adapted models like mixed effect models [77], [42], [43]. In the context of health-care and cost-effectiveness analysis, we are also interested in model of aggregation of different criteria. For this purpose, we develop research about fuzzy binary measures and Choquet integral [63], [81].

3.3. Estimation and control for stochastic processes

When one desires to confront theoretical probabilistic models with real data, statistical tools and control of the dynamics are obviously crucial. As matter of course, we develop inference about stochastic processes that we use for modeling, it is the heart of some of our projects. Control of stochastic processes is also a way to optimise administration (dose, frequency) of therapy.

The monograph [72] is a good reference on the basic estimation techniques for diffusion processes. Some attention has been paid recently to the estimation of the coefficients of fractional or multifractional Brownian motion according to a set of observations. Let us quote for instance the nice surveys [40], [51]. On the other hand, the inference problem for diffusions driven by a fractional Brownian motion has been in its infancy. A good reference on the question is [103], dealing with some very particular families of equations, which do not cover the cases of interest for us. We also recently proposed least-square estimators for these kind of processes [50], [88]. Inference about PDMP is also a recent subject that we want to develop. Our team has a good expertise about inference of the rate jump and the kernel of PDMP [38], [39], [37], [2].

However, there are many directions to go further into. For instance, previous works made the assumption of a complete observation of jumps and mode, that is unrealistic in practice. We want to tackle the problem of inference of "Hidden PDMP". It could be also interesting to investigate estimation followed by optimal control for ergodic PDMP. About pharmacokinetics modeling inference, several papers have been reported for the application of system identification techniques. But two issues were ignored in these previous works: presence of timing noise and identification from longitudinal data. In [41], we have proposed a bounded-error estimation algorithm based on interval analysis to solve the parameter estimation problem while taking into consideration uncertainty on observation time instants. Statistical inference from longitudinal data based on mixed effects models [77] can be performed by the *Monolix* software (http://lixoft.com/products/monolix/) developed by the Monolix group chaired by Marc Lavielle and France Mentré, and supported by Inria. We used it to estimate tumor growth in [42].

We consider the control of stochastic processes within the framework of Markov Decision Processes [90] and their generalization known as multi-player stochastic games [102], with a particular focus on infinite-horizon problems. In this context, we are interested in the complexity analysis of standard algorithms, as well as the proposition and analysis of numerical approximate schemes for large problems in the spirit of [45]. Regarding complexity, a central topic of research is the analysis of the Policy Iteration algorithm, which has made significant progress in the last years [108], [89], [66], [57], [101], but is still not fully understood. For large problems, we have a long experience of sensitivity analysis of approximate dynamic programming algorithms for Markov Decision Processes [99], [98], [100], [79], [97], and we currently investigate whether/how similar ideas may be adapted to multi-player stochastic games.

3.4. Algorithms and estimation for graph data

A graph data structure consists of a set of nodes, together with a set of (either unordered or ordered) pairs of these nodes called edges. This type of data is frequently used in various domains of application (in particular in biology) because they provide a mathematical representation of many concepts such as physical or biological structures and networks of relationship in a population. Some attention has recently been focused in the group on modeling and inference for graph data.

Suppose that we know the value of p variables on n subjects (in many applications, we have $n \ll p$). Inference network consists in evaluating the link between two variables knowing the others. [106] gives a very good introduction and many references about network inference and mining. Gaussian Graphical model is a convenient framework to infer network between quantitative variables: there is a edge between two variables if the partial correlation between them is non zero. So the problem is to compute the partial correlations trough the concentration matrix. Many methods are available to infer and test partial correlations in the context $n \ll p$ [106], [82], [60], [62]. However, when dealing with abundance data, because inflated zero data, data are far from gaussian assumption. Some authors work only with the binary "presence-absence" indicator via log-linear [65]. Models for inflated zero variables are not used for network inference and we want to develop them.

Among graphs, trees play a special role because they offer a good model for many biological concepts, from RNA to phylogenetic trees through plant structures. Our research deals with several aspects of tree data. In particular, we work on statistical inference for this type of data under a given stochastic model (critical Galton-Watson trees for example): in this context, the structure of the tree depends on an integer-valued distribution that we estimate from the observation of either only one tree, or a forest. We also work on lossy compression of trees via linear directed acyclic graphs. These methods make us able to compute distances between tree data faster than from the original structures and with a high accuracy. These results are valuable in the context of very large trees arising for instance in biology of plants.

3.5. Regression and machine learning

Regression models or machine learning aim at inferring statistical links between a variable of interest and covariates. It also aims at clustering subjects or variables in set homogeneous sets. In biological study, it is always important to develop adapted learning methods both in the context of "standard" data and also for very massive or online data.

A first approach for regression of quantitative variable is the non-parametric estimation of its cumulative distribution function. Many methods are available to estimate conditional quantiles and test dependencies [86], [70]. Among them we have developped nonparametric estimation trough local analysis via polynomial [58], [59] and we want to study properties of this estimator in order to derive measure of risk like confidence band and test. We study also many other regression models like survival analysis, spatio temporal models with covariates. Among the multiple regression models, we want to test, thanks to simulation methods, validity of their assumptions. Tests of this kind are called omnibus test. An omnibus test is an overall test that examines several assumptions together, the most known omnibus test is the one for testing gaussianity (that examines both skewness and kurtosis [55]).

As it concerns the analysis point of high dimensional data, our view on the topic relies on the so-called *French data analysis school*, and more specifically on Factorial Analysis tools. In this context, stochastic approximation is an essential tool (see Lebart's paper [78]), which allows one to approximate eigenvectors in a stepwise manner. A systematic study of Principal Component and Factorial Analysis has then been lead by Monnez in the series of papers [85], [83], [84], in which many aspects of convergences of online processes are analyzed thanks to the stochastic approximation techniques. BIGS aims at performing accurate classification or clustering by taking advantage of the possibility of updating the information "online" using stochastic approximation algorithms [71]. We focus on several incremental procedures for regression and data analysis like linear and logistic regressions and PCA. We also focus the biological context of high-throughput bioassays in which several hundreds or thousands of biological signals are measured for a posterior analysis. The inference of the modeling conclusions from a sample of wells to the whole population requires to account for the inter-individual variability within the modeling procedure. One solution consists in using mixed effects models but up to now no similar approach exists in the field of dynamical system identification. As a consequence, we aim at developing a new solution based on an ARX (Auto Regressive model with eXternal inputs) model structure using the EM (Expectation-Maximisation) algorithm for the estimation of the model parameters.

BIOCORE Project-Team

3. Research Program

3.1. Mathematical and computational methods

BIOCORE's action is centered on the mathematical modeling of biological systems, more particularly of artificial ecosystems, that have been built or strongly shaped by human. Indeed, the complexity of such systems where life plays a central role often makes them impossible to understand, control, or optimize without such a formalization. Our theoretical framework of choice for that purpose is Control Theory, whose central concept is "the system", described by state variables, with inputs (action on the system), and outputs (the available measurements on the system). In modeling the ecosystems that we consider, mainly through ordinary differential equations, the state variables are often population, substrate and/or food densities, whose evolution is influenced by the voluntary or involuntary actions of man (inputs and disturbances). The outputs will be some product that one can collect from this ecosystem (harvest, capture, production of a biochemical product, etc), or some measurements (number of individuals, concentrations, etc). Developing a model in biology is however not straightforward: the absence of rigorous laws as in physics, the presence of numerous populations and inputs in the ecosystems, most of them being irrelevant to the problem at hand, the uncertainties and noise in experiments or even in the biological interactions require the development of dedicated techniques to identify and validate the structure of models from data obtained by or with experimentalists.

Building a model is rarely an objective in itself. Once we have checked that it satisfies some biological constraints (eg. densities stay positive) and fitted its parameters to data (requiring tailor-made methods), we perform a mathematical analysis to check that its behavior is consistent with observations. Again, specific methods for this analysis need to be developed that take advantage of the structure of the model (eg. the interactions are monotone) and that take into account the strong uncertainty that is linked to life, so that qualitative, rather than quantitative, analysis is often the way to go.

In order to act on the system, which often is the purpose of our modeling approach, we then make use of two strong points of Control Theory: 1) the development of observers, that estimate the full internal state of the system from the measurements that we have, and 2) the design of a control law, that imposes to the system the behavior that we want to achieve, such as the regulation at a set point or optimization of its functioning. However, due to the peculiar structure and large uncertainties of our models, we need to develop specific methods. Since actual sensors can be quite costly or simply do not exist, a large part of the internal state often needs to be re-constructed from the measurements and one of the methods we developed consists in integrating the large uncertainties by assuming that some parameters or inputs belong to given intervals. We then developed robust observers that asymptotically estimate intervals for the state variables [73]. Using the directly measured variables and those that have been obtained through such, or other, observers, we then develop control methods that take advantage of the system structure (linked to competition or predation relationships between species in bioreactors or in the trophic networks created or modified by biological control).

3.2. A methodological approach to biology: from genes to ecosystems

One of the objectives of BIOCORE is to develop a methodology that leads to the integration of the different biological levels in our modeling approach: from the biochemical reactions to ecosystems. The regulatory pathways at the cellular level are at the basis of the behavior of the individual organism but, conversely, the external stresses perceived by the individual or population will also influence the intracellular pathways. In a modern "systems biology" view, the dynamics of the whole biosystem/ecosystem emerge from the interconnections among its components, cellular pathways/individual organisms/population. The different scales of size and time that exist at each level will also play an important role in the behavior of the biosystem/ecosystem. We intend to develop methods to understand the mechanisms at play at each level, from cellular pathways to individual organisms and populations; we assess and model the interconnections and influence between two scale levels (eg., metabolic and genetic; individual organism and population); we explore the possible regulatory and control pathways between two levels; we aim at reducing the size of these large models, in order to isolate subsystems of the main players involved in specific dynamical behaviors.

We develop a theoretical approach of biology by simultaneously considering different levels of description and by linking them, either bottom up (scale transfer) or top down (model reduction). These approaches are used on modeling and analysis of the dynamics of populations of organisms; modeling and analysis of small artificial biological systems using methods of systems biology; control and design of artificial and synthetic biological systems, especially through the coupling of systems.

The goal of this multi-level approach is to be able to design or control the cell or individuals in order to optimize some production or behavior at higher level: for example, control the growth of microalgae via their genetic or metabolic networks, in order to optimize the production of lipids for bioenergy at the photobioreactor level.

BIOVISION Team

3. Research Program

3.1. Introduction

The Biovision team has started on January 1st, 2016. It aims at developing fundamental research as well as technological developments along two axes.

3.1.1. Axis 1: High tech vision aid systems for low vision patients

The most popular class of vision aid systems for low vision patients is based on the idea of magnification. These aids are helpful for tasks such as reading but of course are not useful in other common daily tasks such as navigation.

Video goggles [0] are another kind of device where visual information is captured by a head-mounted camera, processed and then displayed on a near-the-eye display screen. So far, this technology did not encountered a big success essentially due to their narrow field of view. This situation could evolve with the fast progression of technology around virtual reality and augmented reality.

In BIOVISION we mainly focus on this technology to develop new vision aid systems that could take into account the pathologies of low vision patients but also on the tasks performed by the patients. We have three main goals:

1. We plan to focus on three tasks: reading, watching movies and navigating (indoor or outdoor), which are all important daily life activities for patients.
2. We aim at proposing new **scene enhancements** depending on **pathologies**.
3. We want to test them in **immersive** environments with low vision patients, taking into consideration **ergonomics**.

3.1.2. Axis 2: Human vision understanding through joint experimental and modeling studies, for normal and distrophic retinas

A holistic point of view is emerging in neuroscience where one can observe simultaneously how vision works at different levels of the hierarchy in the visual system. Multiple scales functional analysis and connectomics are also exploding in brain science, and studies of visual systems are upfront on this fast move. These integrated studies call for new classes of theoretical and integrated models where the goal is the modeling of visual functions such as motion integration.

In BIOVISION we contribute to a better understanding of the visual system with three main goals:

1. We aim at proposing simplified mathematical models characterizing how the **retina** converts a visual scene into spike **population coding**, in **normal and under specific pathological conditions**.
2. We want to design an integrated numerical model of the visual stream, with a focus on motion integration, from retina to **visual cortex** area (e.g., the motion stream **V1-MT-MST**).
3. We plan to develop a simulation platform emulating the retinal spike-response to visual and prosthetic simulations, in normal and pathological conditions.

Finally, although this is not the main goal of our team, another natural avenue of our research will be to develop novel synergistic solutions to solve computer vision tasks based on bio-inspired mechanisms.

3.2. Scientific methodology

In this section we briefly describe the scientific methods we use to achieve our research goals.

[0] Video goggles are marketed by several companies such as, e.g., `eSight`, `Enhanced Vision` and `Lumus`

3.2.1. Adaptive image processing

An impressive range of techniques have been developed in the fields of image processing, computer vision and computer graphics to manipulate and interpret image content for a variety of applications. So far only a few of these techniques have been applied in the context of vision aid systems and even less have been carefully evaluated with patients. However it is worth noticing a recent gain of interest from the artificial vision side to low vision applications [0]. We investigate which techniques could bring a real interest for vision aid systems, how to combine them and how to make them adapted to patient needs, so that they can not only "see" an image but understand it more efficiently.

Some techniques have already been explored. Among the first, enhancing image content (equalization, gamma correction, tone mapping, edge enhancement, image decomposition, cartoonization) seems a natural type of processing to make. Some methods have already been tested with low vision patients [38], [54], [55] or even in retina prosthesis systems as a pre-processing [37]. For some visual impairement it can be useful to consider methods that help patients to focus on the most relevant information, using techniques such as scene retargeting [59], seam carving [40], [39], saliency-based enhancements [71], [82] or 3D-based enhancements when available [64]. All the work done on image understanding could also be extremely useful to help patients navigate in natural cluttered environments both in low vision condition or for prosthetics vision [58]. 3D information, obtained from stereo head systems or RGB-D cameras also bring useful information about the environment [62] and integrated systems combining different expertise are appearing [46].

Our goal will be to take the most of state-of-the-art computer vision methods, in combination with virtual and augmented reality devices (Sec. 3.2.2) to provide patients vision aid system that can adapt to their impairment and so that they can easily change the parameters of the processing in an intuitive way.

3.2.2. Virtual and augmented reality

Our goal is to develop vision-aid systems using virtual and augmented reality [87]. There is a rich continuum of devices between virtual reality (which is *a priori* simpler to use since there is no problem of mobility and environment is well defined), and augmented reality (where information has to be superimposed in real time on top of the real environment to enrich it). Between these two extremes, new hybrid see-through systems are available or under development such as light glasses where additional information can be locally displayed at the center or on the corner (e.g., Google glass improving it). We invest on these technologies which enable new kinds of interaction with visual content which could be very powerful when adapted to low vision patients who want to use their remaining sight. We investigate how low vision patients could take benefits from this technology in their daily life activities [47] [0].

We focus on three activities: reading, watching movies and navigating in real world (indoor and outdoor). In these three scenario, this technology should offer crucial advantages for people in low vision. For reading, this could help them solving the page navigation problem or the limitations of magnification encountered when standard CCTVs are used. When watching a movie, the possibility to explore a pre-processed visual scene presented with very high visual angle can help patients to follow the storyline more easily and this poses some interesting questions on the creation of content specifically for virtual reality headsets. Finally, in real scenarios, augmented reality offers promising perspectives to enrich the scene by highly visible visual cues to facilitate low vision patients navigation. Of course the choices of adaptive image processing techniques (see Sec. 3.2.1) will be crucial and this will be the add-on value of our work.

[0] See, e.g., the Special issue on Assistive Computer Vision and Robotics - "Assistive Solutions for Mobility, Communication and HMI" from Computer Vision and Image Understanding (August 2016) or the International Workshop on Assistive Computer Vision and Robotics (ECCV 2016 Sattelite workshop)

[0] Note that wearing such headsets may not be easily accepted by patients who do not want to advertise their disability. More generally, this poses the general question of how users come to accept and use a technology. This question is debated in the Technology Acceptance Model (TAM) which postulates that two specific perceptions about technology determine one behavioral intention to use a technology: perceived ease of use and perceived usefulness (see, e.g., [50]).

Another important aspect of this work that will progressively need attention is ergonomic which will have to take into account the other potential functional limitations of these patients in addition to low vision (e.g., limitations in mobility, hearing, or agility).

3.2.3. Biophysical modeling

Modeling in neuroscience has to cope with several competing objective. On one hand describing the biological realm as close as possible, and, on the other hand, providing tractable equations at least at the descriptive level (simulation, qualitative description) and, when possible, at the mathematical level (i.e., affording a rigorous description). These objectives are rarely achieved simultaneously and most of the time one has to make compromises. In Biovision team we adopt the point of view of physicists: try to capture the phenomenological description of a biophysical mechanism, removing irrelevant details in the description, and try to have a qualitative description of equations behaviour at least at the numerical simulation level, and, when possible, get out analytic results. We do not focus on mathematical proofs, instead insisting on the quality of the model in predicting, and, if possible proposing new experiments. This requires a constant interaction with neuroscientists so as to keep the model on the tracks, warning of too crude approximation, still trying to construct equations from canonical principles [4],[33], [22].

3.2.4. Methods from theoretical physics

Biophysical models mainly consist of differential equations (ODEs or PDEs) or integro-differential equations (neural fields). We study them using dynamical systems and bifurcation theory as well as techniques coming from nonlinear physics (amplitude equations, stability analysis, Lyapunov spectrum, correlation analysis, multi-scales methods).

For the study of large scale populations (e.g., when studying population coding) we use methods coming from statistical physics. This branch of physics gave birth to mean-field methods as well statistical methods for large population analysis. We use both of them. Mean-field methods will be applied for large scale activity in the retina and in the cortex [7], [11],[15].

For the study of retina population coding we use the so-called Gibbs distribution, initially introduced by Boltzmann and Gibbs. This concept includes, but *is not limited to*, maximum entropy models [60] used by numerous authors in the context of the retina (see, e.g., [73], [75], [57], [56], [78]). These papers were restricted to a statistical description without memory neither causality: the time correlations between successive times is not considered. A paradigmatic example of this is the Ising model, used to describe the retinal activity in, e.g., [73], [75]. However, maximum entropy extends to spatio-temporal correlations as we have shown in, e.g., [13], [5].

More generally, while maximum entropy models rely heavily on the questionable assumption of stationariy, the concept of Gibbs distribution does not need this hypothesis. Beside, it allows to handle models with large memory; it also provides a framework to model anticipation [16]. It includes as well existing models to explain retina statistics such as the Generalized Linear Model (GLM) [44].

BONSAI Project-Team

3. Research Program

3.1. Sequence processing for Next Generation Sequencing

As said in the introduction of this document, biological sequence analysis is a foundation subject for the team. In the last years, sequencing techniques have experienced remarkable advances with Next Generation Sequencing (NGS), that allow for fast and low-cost acquisition of huge amounts of sequence data, and outperforms conventional sequencing methods. These technologies can apply to genomics, with DNA sequencing, as well as to transcriptomics, with RNA sequencing. They promise to address a broad range of applications including: Comparative genomics, individual genomics, high-throughput SNP detection, identifying small RNAs, identifying mutant genes in disease pathways, profiling transcriptomes for organisms where little information is available, researching lowly expressed genes, studying the biodiversity in metagenomics. From a computational point of view, NGS gives rise to new problems and gives new insight on old problems by revisiting them: Accurate and efficient remapping, pre-assembling, fast and accurate search of non exact but quality labeled reads, functional annotation of reads, ...

3.2. Noncoding RNA

Our expertise in sequence analysis also applies to noncoding RNA. Noncoding RNA plays a key role in many cellular processes. First examples were given by microRNAs (miRNAs) that were initially found to regulate development in *C. elegans*, or small nucleolar RNAs (snoRNAs) that guide chemical modifications of other RNAs in mammals. Hundreds of miRNAs are estimated to be present in the human genome, and computational analysis suggests that more than 20% of human genes are regulated by miRNAs. To go further in this direction, the 2007 ENCODE Pilot Project provides convincing evidence that the Human genome is pervasively transcribed, and that a large part of this transcriptional output does not appear to encode proteins. All those observations open a universe of “RNA dark matter” that must be explored. From a combinatorial point of view, noncoding RNAs are complex objects. They are single stranded nucleic acid sequences that can fold forming long-range base pairings. This implies that RNA structures are usually modeled by complex combinatorial objects, such as ordered labeled trees, graphs or arc-annotated sequences.

3.3. Genome structures

Our third application domain is concerned with the structural organization of genomes. Genome rearrangements are able to change genome architecture by modifying the order of genes or genomic fragments. The first studies were based on linkage maps and fifteen year old mathematical models. But the usage of computational tools was still limited due to the lack of data. The increasing availability of complete and partial genomes now offers an unprecedented opportunity to analyze genome rearrangements in a systematic way and gives rise to a wide spectrum of problems: Taking into account several kinds of evolutionary events, looking for evolutionary paths conserving common structure of genomes, dealing with duplicated content, being able to analyze large sets of genomes even at the intraspecific level, computing ancestral genomes and paths transforming these genomes into several descendant genomes.

3.4. Nonribosomal peptides

Lastly, the team has been developing for several years a tight collaboration with ProBioGEM team in Institut Charles Viollette on nonribosomal peptides, and has became a leader on that topic. Nonribosomal peptide synthesis produces small peptides not going through the central dogma. As the name suggests, this synthesis uses neither messenger RNA nor ribosome but huge enzymatic complexes called nonribosomal peptide synthetases (NRPSs). This alternative pathway is found typically in bacteria and fungi. It has been described for the first time in the 70's. For the last decade, the interest in nonribosomal peptides and their synthetases has considerably increased, as witnessed by the growing number of publications in this field. These peptides are or can be used in many biotechnological and pharmaceutical applications (e.g. anti-tumors, antibiotics, immuno-modulators).

CAMIN Team

3. Research Program

3.1. Exploration and understanding of the origins and control of movement

One of CAMIN's areas of expertise is **motion measurement, observation and modeling** in the context of **sensorimotor deficiencies**. The team has the capacity to design advanced protocols to explore motor control mechanisms in more or less invasive conditions in both animal and human.

Human movement can be assessed by several noninvasive means, from motion observation (MOCAP, IMU) to electrophysiological measurements (afferent ENG, EMG, see below). Our general approach is to develop solutions that are realistic in terms of clinical or home use by clinical staff and/or patients for diagnosis and assessment purposes. In doing so, we try to gain a better understanding of motor control mechanisms, including deficient ones, which in turn will give us greater insight into the basics of human motor control. Our ultimate goal is to optimally match a neuroprosthesis to the targeted sensorimotor deficiency.

The team is involved in research projects including:

- Peripheral nervous system (PNS) exploration, modeling and electrophysiology techniques
  Electroneurography (ENG) and electromyography (EMG) signals inform about neural and muscular activities. The team investigates both natural and evoked ENG/EMG through advanced and dedicated signal processing methods. Evoked responses to ES are very precious information for understanding neurophysiological mechanisms, as both the input (ES) and the output (evoked EMG/ENG) are controlled. CAMIN has the expertise to perform animal experiments (rabbits, rats, earthworms and big animals with partners), design hardware and software setups to stimulate and record in harsh conditions, process signals, analyze results and develop models of the observed mechanisms. Experimental surgery is mandatory in our research prior to invasive interventions in humans. It allows us to validate our protocols from theoretical, practical and technical aspects.
- Central nervous system (CNS) exploration
  Stimulating the CNS directly instead of nerves allows activation of the neural networks responsible for generating functions. Once again, if selectivity is achieved the number of implanted electrodes and cables would be reduced, as would the energy demand. We have investigated **spinal electrical stimulation** in animals (pigs) for urinary track and lower limb function management. This work is very important in terms of both future applications and the increase in knowledge about spinal circuitry. The challenges are technical, experimental and theoretical, and the preliminary results have enabled us to test some selectivity modalities through matrix electrode stimulation. This research area will be further intensified in the future as one of ways to improve neuroprosthetic solutions.
  We intend to gain a better understanding of the electrophysiological effects of DES through electroencephalographic (EEG) and electrocorticographic (ECoG) recordings in order to optimize anatomo-functional brain mapping, better understand brain dynamics and plasticity, and improve surgical planning, rehabilitation, and the quality of life of patients.
- Muscle models and fatigue exploration
  Muscle fatigue is one of the major limitations in all FES studies. Simply, the muscle torque varies over time even when the same stimulation pattern is applied. As there is also muscle recovery when there is a rest between stimulations, modeling the fatigue is almost an impossible task. Therefore, it is essential to monitor the muscle state and assess the expected muscle response by FES to improve the current FES system in the direction of greater adaptive force/torque control in the presence of muscle fatigue.
- Movement interpretation

We intend to develop ambulatory solutions to allow ecological observation. We have extensively investigated the possibility of using inertial measurement units (IMUs) within body area networks to observe movement and assess posture and gait variables. We have also proposed extracting gait parameters like stride length and foot-ground clearance for evaluation and diagnosis purposes.

3.2. Movement assistance and/or restoration

The challenges in movement restoration are: (i) improving nerve/muscle stimulation modalities and efficiency and (ii) global management of the function that is being restored in interaction with the rest of the body under voluntary control. For this, both local (muscle) and global (function) controls have to be considered.
Online modulation of ES parameters in the context of lower limb functional assistance requires the availability of information about the ongoing movement. Different levels of complexity can be considered, going from simple open-loop to complex control laws (figure 2).

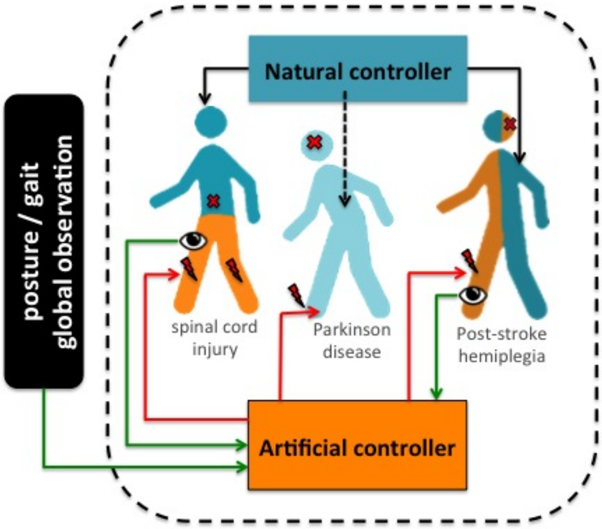


Figure 2. FES assistance should take into account the coexistence of artificial and natural controllers. Artificial controllers should integrate both global (posture/gait) and local (limb/joint) observations.

Real-time adaptation of the stimulation patterns is an important challenge in most of the clinical applications we consider. The modulation of ES parameters in the presence of fatigue or to adapt to context needs for adaptive controllers processing information on movement execution and environmental changes. A minimum number of sensors with minimal impact on patient motion is necessary.

CAPSID Project-Team

3. Research Program

3.1. Classifying and Mining Protein Structures and Protein Interactions

3.1.1. Context

The scientific discovery process is very often based on cycles of measurement, classification, and generalisation. It is easy to argue that this is especially true in the biological sciences. The proteins that exist today represent the molecular product of some three billion years of evolution. Therefore, comparing protein sequences and structures is important for understanding their functional and evolutionary relationships [66], [44]. There is now overwhelming evidence that all living organisms and many biological processes share a common ancestry in the tree of life. Historically, much of bioinformatics research has focused on developing mathematical and statistical algorithms to process, analyse, annotate, and compare protein and DNA sequences because such sequences represent the primary form of information in biological systems. However, there is growing evidence that structure-based methods can help to predict networks of protein-protein interactions (PPIs) with greater accuracy than those which do not use structural evidence [48], [71]. Therefore, developing techniques which can mine knowledge of protein structures and their interactions is an important way to enhance our knowledge of biology [34].

3.1.2. Quantifying Structural Similarity

Often, proteins may be divided into modular sub-units called domains, which can be associated with specific biological functions. Thus, a protein domain may be considered as the evolutionary unit of biological structure and function [70]. However, while it is well known that the 3D structures of protein domains are often more evolutionarily conserved than their one-dimensional (1D) amino acid sequences, comparing 3D structures is much more difficult than comparing 1D sequences. However, until recently, most evolutionary studies of proteins have compared and clustered 1D amino acid and nucleotide sequences rather than 3D molecular structures.

A pre-requisite for the accurate comparison of protein structures is to have a reliable method for quantifying the structural similarity between pairs of proteins. We recently developed a new protein structure alignment program called Kpax which combines an efficient dynamic programming based scoring function with a simple but novel Gaussian representation of protein backbone shape [59]. This means that we can now quantitatively compare 3D protein domains at a similar rate to throughput to conventional protein sequence comparison algorithms. We recently compared Kpax with a large number of other structure alignment programs, and we found Kpax to be the fastest and amongst the most accurate, in a CATH family recognition test [50]. The latest version of Kpax [20] can calculate multiple flexible alignments, and thus promises to avoid such issues when comparing more distantly related protein folds and fold families.

3.1.3. Formalising and Exploiting Domain Knowledge

Concerning protein structure classification, we aim to explore novel classification paradigms to circumvent the problems encountered with existing hierarchical classifications of protein folds and domains. In particular it will be interesting to set up fuzzy clustering methods taking advantage of our previous work on gene functional classification [36], but instead using Kpax domain-domain similarity matrices. A non-trivial issue with fuzzy clustering is how to handle similarity rather than mathematical distance matrices, and how to find the optimal number of clusters, especially when using a non-Euclidean similarity measure. We will adapt the algorithms and the calculation of quality indices to the Kpax similarity measure. More fundamentally, it will be necessary to integrate this classification step in the more general process leading from data to knowledge called Knowledge Discovery in Databases (KDD) [40].

Another example where domain knowledge can be useful is during result interpretation: several sources of knowledge have to be used to explicitly characterise each cluster and to help decide its validity. Thus, it will be useful to be able to express data models, patterns, and rules in a common formalism using a defined vocabulary for concepts and relationships. Existing approaches such as the Molecular Interaction (MI) format [45] developed by the Human Genome Organization (HUGO) mostly address the experimental wet lab aspects leading to data production and curation [55]. A different point of view is represented in the Interaction Network Ontology (INO; http://www.ino-ontology.org/) which is a community-driven ontology that is being developed to standardise and integrate data on interaction networks and to support computer-assisted reasoning [72]. However, this ontology does not integrate basic 3D concepts and structural relationships. Therefore, extending such formalisms and symbolic relationships will be beneficial, if not essential, when classifying the 3D shapes of proteins at the domain family level.

3.1.4. 3D Protein Domain Annotation and Shape Mining

A widely used collection of protein domain families is “Pfam” [39], constructed from multiple alignments of protein sequences. Integrating domain-domain similarity measures with knowledge about domain binding sites, as introduced by us in our KBDOCK approach [1], [3], can help in selecting interesting subsets of domain pairs before clustering. Thanks to our KBDOCK and Kpax projects, we already have a rich set of tools with which we can start to process and compare all known protein structures and PPIs according to their component Pfam domains. Linking this new classification to the latest “SIFTS” (Structure Integration with Function, Taxonomy and Sequence) [67] functional annotations between standard Uniprot (http://www.uniprot.org/ sequence identifiers and protein structures from the Protein Data Bank (PDB) [33] could then provide a useful way to discover new structural and functional relationships which are difficult to detect in existing classification schemes such as CATH or SCOP. As part of the thesis project of Seyed Alborzi, we have developed a recommender-based data mining technique to associate enzyme classification code numbers with Pfam domains using our recently developed EC-DomainMiner program [29].

3.2. Integrative Multi-Component Assembly and Modeling

3.2.1. Context

At the molecular level, each PPI is embodied by a physical 3D protein-protein interface. Therefore, if the 3D structures of a pair of interacting proteins are known, it should in principle be possible for a docking algorithm to use this knowledge to predict the structure of the complex. However, modeling protein flexibility accurately during docking is very computationally expensive due to the very large number of internal degrees of freedom in each protein, associated with twisting motions around covalent bonds. Therefore, it is highly impractical to use detailed force-field or geometric representations in a brute-force docking search. Instead, most protein docking algorithms use fast heuristic methods to perform an initial rigid-body search in order to locate a relatively small number of candidate binding orientations, and these are then refined using a more expensive interaction potential or force-field model, which might also include flexible refinement using molecular dynamics (MD), for example.

3.2.2. Polar Fourier Docking Correlations

In our *Hex* protein docking program [60], the shape of a protein molecule is represented using polar Fourier series expansions of the form

$$\sigma(\underline{x}) = \sum_{nlm} a_{nlm} R_{nl}(r) y_{lm}(\theta, \phi), \tag{70}$$

where $\sigma(\underline{x})$ is a 3D shape-density function, a_{nlm} are the expansion coefficients, $R_{nl}(r)$ are orthonormal Gauss-Laguerre polynomials and $y_{lm}(\theta, \phi)$ are the real spherical harmonics. The electrostatic potential, $\phi(\underline{x})$, and charge density, $\rho(\underline{x})$, of a protein may be represented using similar expansions. Such representations allow the *in vacuo* electrostatic interaction energy between two proteins, A and B, to be calculated as [47]

$$E = \frac{1}{2}\int \phi_A(\underline{x})\rho_B(\underline{x})\mathrm{d}\underline{x} + \frac{1}{2}\int \phi_B(\underline{x})\rho_A(\underline{x})\mathrm{d}\underline{x}. \qquad (71)$$

This equation demonstrates using the notion of *overlap* between 3D scalar quantities to give a physics-based scoring function. If the aim is to find the configuration that gives the most favourable interaction energy, then it is necessary to perform a six-dimensional search in the space of available rotational and translational degrees of freedom. By re-writing the polar Fourier expansions using complex spherical harmonics, we showed previously that fast Fourier transform (FFT) techniques may be used to accelerate the search in up to five of the six degrees of freedom [61]. Furthermore, we also showed that such calculations may be accelerated dramatically on modern graphics processor units [9], [6]. Consequently, we are continuing to explore new ways to exploit the polar Fourier approach.

3.2.3. Assembling Symmetrical Protein Complexes

Although protein-protein docking algorithms are improving [62], [49], it still remains challenging to produce a high resolution 3D model of a protein complex using *ab initio* techniques, mainly due to the problem of structural flexibility described above. However, with the aid of even just one simple constraint on the docking search space, the quality of docking predictions can improve dramatically [61][9]. In particular, many protein complexes involve symmetric arrangements of one or more sub-units, and the presence of symmetry may be exploited to reduce the search space considerably [32], [58], [65]. For example, using our operator notation (in which $\widehat{R}$ and $\widehat{T}$ represent 3D rotation and translation operators, respectively), we have developed an algorithm which can generate and score candidate docking orientations for monomers that assemble into cyclic (C_n) multimers using 3D integrals of the form

$$E_{AB}(y,\alpha,\beta,\gamma) = \int \left[\widehat{T}(0,y,0)\widehat{R}(\alpha,\beta,\gamma)\phi_A(\underline{x})\right] \times \left[\widehat{R}(0,0,\omega_n)\widehat{T}(0,y,0)\widehat{R}(\alpha,\beta,\gamma)\rho_B(\underline{x})\right] \mathrm{d}\underline{x}, \qquad (72)$$

where the identical monomers A and B are initially placed at the origin, and $\omega_n = 2\pi/n$ is the rotation about the principal n-fold symmetry axis. This example shows that complexes with cyclic symmetry have just 4 rigid body degrees of freedom (DOFs), compared to $6(n-1)$ DOFs for non-symmetrical n-mers. We have generalised these ideas in order to model protein complexes that crystallise into any of the naturally occurring point group symmetries (C_n, D_n, T, O, I). This approach was published in 2016 [19], and was subsequently applied to several symmetrical complexes from the “CAPRI” blind docking experiment [13]. Although we currently use shape-based FFT correlations, the symmetry operator technique may equally be used to refine candidate solutions using a more accurate coarse-grained (CG) force-field scoring function.

3.2.4. Coarse-Grained Models

Many approaches have been proposed in the literature to take into account protein flexibility during docking. The most thorough methods rely on expensive atomistic simulations using MD. However, much of a MD trajectory is unlikely to be relevant to a docking encounter unless it is constrained to explore a putative protein-protein interface. Consequently, MD is normally only used to refine a small number of candidate rigid body docking poses. A much faster, but more approximate method is to use CG normal mode analysis (NMA) techniques to reduce the number of flexible degrees of freedom to just one or a handful of the most significant vibrational modes [54], [37], [51], [52]. In our experience, docking ensembles of NMA conformations does not give much improvement over basic FFT-based soft docking [68], and it is very computationally expensive to use side-chain repacking to refine candidate soft docking poses [2].

In the last few years, CG *force-field* models have become increasingly popular in the MD community because they allow very large biomolecular systems to be simulated using conventional MD programs [31]. Typically, a CG force-field representation replaces the atoms in each amino acid with from 2 to 4 “pseudo-atoms”, and it assigns each pseudo-atom a small number of parameters to represent its chemo-physical properties. By directly attacking the quadratic nature of pair-wise energy functions, coarse-graining can speed up MD simulations by up to three orders of magnitude. Nonetheless, such CG models can still produce useful models of very large multi-component assemblies [64]. Furthermore, this kind of coarse-graining effectively integrates out many of the internal DOFs to leave a smoother but still physically realistic energy surface [46]. We are therefore developing a “coarse-grained” scoring function for fast protein-protein docking and multi-component assembly in the frame of the PhD project of Maria-Elisa Ruiz-Echartea (commenced November 2016).

3.2.5. Assembling Multi-Component Complexes and Integrative Structure Modeling

We also want to develop related approaches for integrative structure modeling using cryo-electron microscopy (cryo-EM). Thanks to recently developments in cryo-EM instruments and technologies, its is now feasible to capture low resolution images of very large macromolecular machines. However, while such developments offer the intriguing prospect of being able to trap biological systems in unprecedented levels of detail, there will also come an increasing need to analyse, annotate, and interpret the enormous volumes of data that will soon flow from the latest instruments. In particular, a new challenge that is emerging is how to fit previously solved high resolution protein structures into low resolution cryo-EM density maps. However, the problem here is that large molecular machines will have multiple sub-components, some of which will be unknown, and many of which will fit each part of the map almost equally well. Thus, the general problem of building high resolution 3D models from cryo-EM data is like building a complex 3D jigsaw puzzle in which several pieces may be unknown or missing, and none of which will fit perfectly. Although we do not have precise road-map to a solution for the multi-component assembly problem, we wish to proceed firstly by putting more emphasis on the single-body terms in the scoring function, and secondly by using fast CG representations and knowledge-based distance restraints to prune large regions of the search space.

CARMEN Project-Team

3. Research Program

3.1. Complex models for the propagation of cardiac action potentials

The contraction of the heart is coordinated by a complex electrical activation process which relies on about a million ion channels, pumps, and exchangers of various kinds in the membrane of each cardiac cell. Their interaction results in a periodic change in transmembrane potential called an action potential. Action potentials in the cardiac muscle propagate rapidly from cell to cell, synchronizing the contraction of the entire muscle to achieve an efficient pump function. The spatio-temporal pattern of this propagation is related both to the function of the cellular membrane and to the structural organization of the cells into tissues. Cardiac arrythmias originate from malfunctions in this process. The field of cardiac electrophysiology studies the multiscale organization of the cardiac activation process from the subcellular scale up to the scale of the body. It relates the molecular processes in the cell membranes to the propagation process and to measurable signals in the heart and to the electrocardiogram, an electrical signal on the torso surface.

Several improvements of current models of the propagation of the action potential are developed, based on previous work [44] and on the data available at IHU LIRYC:

- Enrichment of the current monodomain and bidomain models [44] [8] by accounting for structural heterogeneities of the tissue at an intermediate scale. Here we focus on multiscale analysis techniques applied to the various high-resolution structural data available at the LIRYC.
- Coupling of the tissues from the different cardiac compartments and conduction systems. Here, we develop models that couple 1D, 2D and 3D phenomena described by reaction-diffusion PDEs.

These models are essential to improve our in-depth understanding of cardiac electrical dysfunction. To this aim, we use high-performance computing techniques in order to numerically explore the complexity of these models.

We use these model codes for applied studies in two important areas of cardiac electrophysiology: atrial fibrillation [20] [46] and sudden-cardiac-death (SCD) syndromes [14], [51], [48]. This work is performed in collaboration with several physiologists and clinicians both at IHU Liryc and abroad.

3.2. Simplified models and inverse problems

The medical and clinical exploration of the cardiac electric signals is based on accurate reconstruction of the patterns of propagation of the action potential. The correct detection of these complex patterns by non-invasive electrical imaging techniques has to be developed. This problem involves solving inverse problems that cannot be addressed with the more compex models. We want both to develop simple and fast models of the propagation of cardiac action potentials and improve the solutions to the inverse problems found in cardiac electrical imaging techniques.

The cardiac inverse problem consists in finding the cardiac activation maps or, more generally, the whole cardiac electrical activity, from high-density body surface electrocardiograms. It is a new and a powerful diagnosis technique, which success would be considered as a breakthrough. Although widely studied recently, it remains a challenge for the scientific community. In many cases the quality of reconstructed electrical potential is not adequate. The methods used consist in solving the Laplace equation on the volume delimited by the body surface and the epicardial surface. Our aim is to

- study in depth the dependance of this inverse problem on inhomogeneities in the torso, conductivity values, the geometry, electrode positions, etc., and
- improve the solution to the inverse problem by using new regularization strategies, factorization of boundary value problems, and the theory of optimal control, both in the quasistatic and in the dynamic contexts.

Of course we will use our models as a basis to regularize these inverse problems. We will consider the following strategies:

- using complete propagation models in the inverse problem, like the bidomain equations, for instance in order to localize electrical sources;
- constructing families of reduced-order models using e.g. statistical learning techniques, which would accurately represent some families of well-identified pathologies; and
- constructing simple models of the propagation of the activation front, based on eikonal or level-set equations, but which would incorporate the representation of complex activation patterns.

Additionaly, we will need to develop numerical techniques dedicated to our simplified eikonal/level-set equations.

3.3. Numerical techniques

We want the numerical simulations of the previous direct or inverse models to be efficient and reliable with respect to the needs of the medical community. They should qualify and guarantee the accuracy and robustness of the numerical techniques and the efficiency of the resolution algorithms.

Based on previous work on solving the monodomain and bidomain equations [4], [5], [7], [1], we will focus on

- High-order numerical techniques with respect to the variables with physiological meaning, like velocity, AP duration and restitution properties.
- Efficient, dedicated preconditioning techniques coupled with parallel computing.

Existing simulation tools used in our team rely, among others, on mixtures of explicit and implicit integration methods for ODEs, hybrid MPI-OpenMP parallellization, algebraic multigrid preconditioning, and a BiCGStab algorithm with adaptations to retain numerical accuracy while handling large underdetermined systems.

3.4. Cardiac Electrophysiology at the Microscopic Scale

Numerical models of whole-heart physiology are based on the approximation of a perfect muscle using homogenisation methods. However, due to aging and cardiomyopathies, the cellular structure of the tissue changes. These modifications can give rise to life-threatening arrhythmias. For our research on this subject and with cardiologists of the IHU LIRYC Bordeaux, we aim to design and implement models that describe the strong heterogeneity of the tissue at the cellular level and to numerically explore the mechanisms of these diseases.

The literature on this type of model is still very limited. Existing models are two-dimensional or limited to idealized geometries, and use a linear (purely resistive) behaviour of the gap-juction channels that connect the cells. We propose a three-dimensional approach using realistic cellular geometry, nonlinear gap-junction behaviour, and a numerical approach that can scale to hundreds of cells while maintaining a sub-micrometer spatial resolution (10 to 100 times smaller than the size of a cardiomyocyte).

CASTOR Project-Team

3. Research Program

3.1. Plasma Physics

Participants: Jacques Blum, Cédric Boulbe, Blaise Faugeras, Hervé Guillard, Holger Heumann, Sebastian Minjeaud, Boniface Nkonga, Richard Pasquetti, Afeintou Sangam.

The main reseach topics are:

1. Modelling and analysis
   - Fluid closure in plasma
   - Turbulence
   - Plasma anisotropy type instabilities
   - Free boundary equilibrium (FBE)
   - Coupling FBE – Transport
2. Numerical methods and simulations
   - High order methods
   - Curvilinear coordinate systems
   - Equilibrium simulation
   - Pressure correction scheme
   - Anisotropy
   - Solving methods and parallelism
3. Identification and control
   - Inverse problem: Equilibrium reconstruction
   - Open loop control
4. Applications
   - MHD instabilities : Edge-Localized Modes (ELMs)
   - Edge plasma turbulence
   - Optimization of scenarii

CLIME Project-Team

3. Research Program

3.1. Data assimilation and inverse modeling

This activity is one major concern of environmental sciences. It matches up the setting and the use of data assimilation methods, for instance variational methods (such as the 4D-Var method). An emerging issue lies in the propagation of uncertainties by models, notably through ensemble forecasting methods.

Although modeling is not part of the scientific objectives of Clime, the project-team has complete access to air quality models through collaborations with École des Ponts ParisTech and EDF R&D: the models from Polyphemus (pollution forecasting from local to regional scales) and Code_Saturne (urban scale). In regard to other modeling domains, such as oceanography and meteorology, Clime accesses models through co-operation with LOCEAN (Laboratoire d'OCEANographie et du climat, UPMC) and Météo-France.

The research activities of Clime tackle scientific issues such as:

- Within a family of models (differing by their physical formulations and numerical approximations), which is the optimal model for a given set of observations?
- How to reduce dimensionality of problems by Galerkin projection of equations on subspaces? How to define these subspaces in order to keep the main properties of systems?
- How to assess the quality of a forecast and its uncertainty? How do data quality, missing data, data obtained from sub-optimal locations, affect the forecast? How to better include information on uncertainties (of data, of models) within the data assimilation system?
- How to make a forecast (and a better forecast!) by using several models corresponding to different physical formulations? It also raises the question: how should data be assimilated in this context?
- Which observational network should be set up to perform a better forecast, while taking into account additional criteria such as observation cost? What are the optimal location, type and mode of deployment of sensors? How should trajectories of mobile sensors be operated, while the studied phenomenon is evolving in time? This issue is usually referred as "network design".

3.2. Satellite acquisitions and image assimilation

In geosciences, the issue of coupling data, in particular satellite acquisitions, and models is extensively studied for meteorology, oceanography, chemistry-transport and land surface models. However, satellite images are mostly assimilated on a point-wise basis. Three major approaches arise if taking into account the spatial structures, whose displacement is visualized on image sequences:

- Image approach. Image assimilation allows the extraction of features from image sequences, for instance motion field or structures' trajectory. A model of the dynamics is considered (obtained by simplification of a geophysical model such as Navier-Stokes equations). An observation operator is defined to express the links between the model state and the pixel values or some image features. In the simplest case, the pixel value corresponds to one coordinate of the model state and the observation operator is reduced to a projection. However, in most cases, this operator is highly complex, implicit and non-linear. Data assimilation techniques are developed to control the initial state or the whole assimilation window. Image assimilation is also applied to learn reduced models from image data and estimate a reliable and small-size reconstruction of the dynamics, which is observed on the sequence.
- Model approach. Image assimilation is used to control an environmental model and obtain improved forecasts. In order to take into account the spatial and temporal coherency of structures, specific image characteristics are considered and dedicated norms and observation error covariances are defined.

- Correcting a model. Another topic, mainly described for meteorology in the literature, concerns the location of structures. How to force the existence and to correct the location of structures in the model state using image information? Most of the operational meteorological forecasting institutes, such as Météo-France (in France), UK-met (in United Kingdom), KNMI (in Netherlands), ZAMG (in Austria) and Met-No (in Norway), study this issue because operational forecasters often modify their forecasts based on visual comparisons between the model outputs and the structures displayed on satellite images.

3.3. Software chains for environmental applications

An objective of Clime is to participate in the design and creation of software chains for impact assessment and environmental crisis management. Such software chains bring together static or dynamic databases, data assimilation systems, forecast models, processing methods for environmental data and images, complex visualization tools, scientific workflows, ...

Clime is currently building, in partnership with École des Ponts ParisTech and EDF R&D, such a system for air pollution modeling: Polyphemus (see the web site http://cerea.enpc.fr/polyphemus/), whose architecture is specified to satisfy data requirements (e.g., various raw data natures and sources, data preprocessing) and to support different uses of an air quality model (e.g., forecasting, data assimilation, ensemble runs).

COFFEE Project-Team

3. Research Program

3.1. Research Program

Mathematical modeling and computer simulation are among the main research tools for environmental management, risks evaluation and sustainable development policy. Many aspects of the computer codes as well as the PDEs systems on which these codes are based can be considered as questionable regarding the established standards of applied mathematical modeling and numerical analysis. This is due to the intricate multiscale nature and tremendous complexity of those phenomena that require to set up new and appropriate tools. Our research group aims to contribute to bridging the gap by developing advanced abstract mathematical models as well as related computational techniques.

The scientific basis of the proposal is two–fold. On the one hand, the project is “technically–driven”: it has a strong content of mathematical analysis and design of general methodology tools. On the other hand, the project is also “application–driven”: we have identified a set of relevant problems motivated by environmental issues, which share, sometimes in a unexpected fashion, many common features. The proposal is precisely based on the conviction that these subjects can mutually cross-fertilize and that they will both be a source of general technical developments, and a relevant way to demonstrate the skills of the methods we wish to design.

To be more specific:

- We consider evolution problems describing highly heterogeneous flows (with different phases or with high density ratio). In turn, we are led to deal with non linear systems of PDEs of convection and/or convection–diffusion type.
- The nature of the coupling between the equations can be two–fold, which leads to different difficulties, both in terms of analysis and conception of numerical methods. For instance, the system can couple several equations of different types (elliptic/parabolic, parabolic/hyperbolic, parabolic or elliptic with algebraic constraints, parabolic with degenerate coefficients....). Furthermore, the unknowns can depend on different sets of variables, a typical example being the fluid/kinetic models for particulate flows. In turn, the simulation cannot use a single numerical approach to treat all the equations. Instead, hybrid methods have to be designed which raise the question of fitting them in an appropriate way, both in terms of consistency of the discretization and in terms of stability of the whole computation. For the problems under consideration, the coupling can also arises through interface conditions. It naturally occurs when the physical conditions are highly different in subdomains of the physical domain in which the flows takes place. Hence interface conditions are intended to describe the exchange (of mass, energy...) between the domains. Again it gives rise to rather unexplored mathematical questions, and for numerics it yields the question of defining a suitable matching at the discrete level, that is requested to preserve the properties of the continuous model.
- By nature the problems we wish to consider involve many different scales (of time or length basically). It raises two families of mathematical questions. In terms of numerical schemes, the multiscale feature induces the presence of stiff terms within the equations, which naturally leads to stability issues. A clear understanding of scale separation helps in designing efficient methods, based on suitable splitting techniques for instance. On the other hand asymptotic arguments can be used to derive hierarchy of models and to identify physical regimes in which a reduced set of equations can be used.

We can distinguish the following fields of expertise

- Numerical Analysis: Finite Volume Schemes, Well-Balanced and Asymptotic-Preserving Methods
  - Finite Volume Schemes for Diffusion Equations
  - Finite Volume Schemes for Conservation Laws
  - Well-Balanced and Asymptotic-Preserving Methods
- Modeling and Analysis of PDEs
  - Kinetic equations and hyperbolic systems
  - PDEs in random media
  - Interface problems

DRACULA Project-Team

3. Research Program

3.1. Cell dynamics

We model dynamics of cell populations with two approaches, dissipative particle dynamics (DPD) and partial differential equations (PDE) of continuum mechanics. DPD is a relatively new method developed from molecular dynamics approach largely used in statistical physics. Particles in DPD do not necessarily correspond to atoms or molecules as in molecular dynamics. These can be mesoscopic particles. Thus, we describe in this approach a system of particles. In the simplest case where each particle is a sphere, they are characterized by their positions and velocities. The motion of particles is determined by Newton's second law (see Figure 1).

In our case, particles correspond to biological cells. The specific feature of this case in comparison with the conventional DPD is that cells can divide (proliferation), change their type (differentiation) and die by apoptosis or necrosis. Moreover, they interact with each other and with the extra-cellular matrix not only mechanically but also chemically. They can exchange signals, they can be influenced by various substances (growth factors, hormones, nutrients) coming from the extra-cellular matrix and, eventually, from other organs.

Distribution of the concentrations of bio-chemical substances in the extra-cellular matrix will be described by the diffusion equation with or without convective terms and with source and/or sink terms describing their production or consumption by cells. Thus we arrive to a coupled DPD-PDE model.

Cell behaviour (proliferation, differentiation, apoptosis) is determined by intra-cellular regulatory networks, which can be influenced by external signals. Intra-cellular regulatory networks (proteins controlling the cell cycle) can be described by systems of ordinary differential equations (ODE). Hence we obtain DPD-PDE-ODE models describing different levels of cell dynamics (see Figure 1). It is important to emphasize that the ODE systems are associated to each cell and they can depend on the cell environment (extra-cellular matrix and surrounding cells).

3.2. From particle dynamics to continuum mechanics

DPD is well adapted to describe biological cells. However, it is a very time consuming method which becomes difficult to use if the number of particles exceeds the order of 10^5-10^6 (unless distributed computing is used). On the other hand, PDEs of continuum mechanics are essentially more efficient for numerical simulations. Moreover, they can be studied by analytical methods which have a crucial importance for the understanding of relatively simple test cases. Thus we need to address the question about the relation between DPD and PDE. The difficulty follows already from the fact that molecular dynamics with the Lennard-Jones potential can describe very different media, including fluids (compressible, incompressible, non-Newtonian, and so on) and solids (elastic, elasto-plastic, and so on). Introduction of dissipative terms in the DPD models can help to justify the transition to a continuous medium because each medium has a specific to it law of dissipation. Our first results [33] show the correspondence between a DPD model and Darcy's law describing fluid motion in a porous medium. However, we cannot expect a rigorous justification in the general case and we will have to carry out numerical comparison of the two approaches.

An interesting approach is related to hybrid models where PDEs of continuum mechanics are considered in the most part of the domain, where we do not need a microscopical description, while DPD in some particular regions are required to consider individual cells.

3.3. PDE models

If we consider cell populations as a continuous medium, then cell concentrations can be described by reaction-diffusion systems of equations with convective terms. The diffusion terms correspond to a random cell motion and the reaction terms to cell proliferation, differentiation and death. These are more traditional models [36] with properties that depend on the particular problem under consideration and with many open questions, both from the point of view of their mathematical properties and for applications. In particular we are interested in the spreading of cell populations which describes the development of leukemia in the bone marrow and many other biological phenomena (solid tumors, morphogenesis, atherosclerosis, and so on). From the mathematical point of view, these are reaction-diffusion waves, intensively studied in relation with various biological problems. We will continue our studies of wave speed, stability, nonlinear dynamics and pattern formation. From the mathematical point of view, these are elliptic and parabolic problems in bounded or unbounded domains, and integro-differential equations. We will investigate the properties of the corresponding linear and nonlinear operators (Fredholm property, solvability conditions, spectrum, and so on). Theoretical investigations of reaction-diffusion-convection models will be accompanied by numerical simulations and will be applied to study hematopoiesis.

Hyperbolic problems are also of importance when describing cell population dynamics ([42], [46]), and they proved effective in hematopoiesis modelling ([28], [29], [31]). They are structured transport partial differential equations, in which the structure is a characteristic of the considered population, for instance age, size, maturity, protein concentration, etc. The transport, or movement in the structure space, simulates the progression of the structure variable, growth, maturation, protein synthesis, etc. Several questions are still open in the study of transport PDE, yet we will continue our analysis of these equations by focusing in particular on the asymptotic behaviour of the system (stability, bifurcation, oscillations) and numerical simulations of nonlocal transport PDE.

The use of age structure often leads to a reduction (by integration over the age variable) to nonlocal problems [46]. The nonlocality can be either in the structure variable or in the time variable [28]. In particular, when coefficients of an age-structured PDE are not supposed to depend on the age variable, this reduction leads to delay differential equations.

3.4. Delay differential Equations

Delay differential equations (DDEs) are particularly useful for situations where the processes are controlled through feedback loops acting after a certain time. For example, in the evolution of cell populations the transmission of control signals can be related to some processes as division, differentiation, maturation, apoptosis, etc. Because these processes can take a certain time, the system depends on an essential way of its past state, and can be modelled by DDEs.

We explain hereafter how delays can appear in hematopoietic models. Based on biological aspects, we can divide hematopoietic cell populations into many compartments. We basically consider two different cell populations, one composed with immature cells, and the other one made of mature cells. Immature cells are separated in many stages (primitive stem cells, progenitors and precursors, for example) and each stage is composed with two sub-populations, resting (G0) and proliferating cells. On the opposite, mature cells are known to proliferate without going into the resting compartment. Usually, to describe the dynamic of these multi-compartment cell populations, transport equations (hyperbolic PDEs) are used. Structure variables are age and discrete maturity. In each proliferating compartment, cell count is controlled by apoptosis (programmed cell death), and in the other compartments, cells can be eliminated only by necrosis (accidental cell death). Transitions between the compartments are modelled through boundary conditions. In order to reduce the complexity of the system and due to some lack of information, no dependence of the coefficients on cell age is assumed. Hence, the system can be integrated over the age variable and thus, by using the method of characteristics and the boundary conditions, the model reduces to a system of DDEs, with several delays.

Leaving all continuous structures, DDEs appear well adapted to us to describe the dynamics of cell populations. They offer good tools to study the behaviour of the systems. The main investigation of DDEs are the effect of perturbations of the parameters, as cell cycle duration, apoptosis, differentiation, self-renewal, and re-introduction from quiescent to proliferating phase, on the behaviour of the system, in relation for instance with some hematological disorders [38].

DYLISS Project-Team

3. Research Program

3.1. Modeling knowledge integration with combinatorial constraints

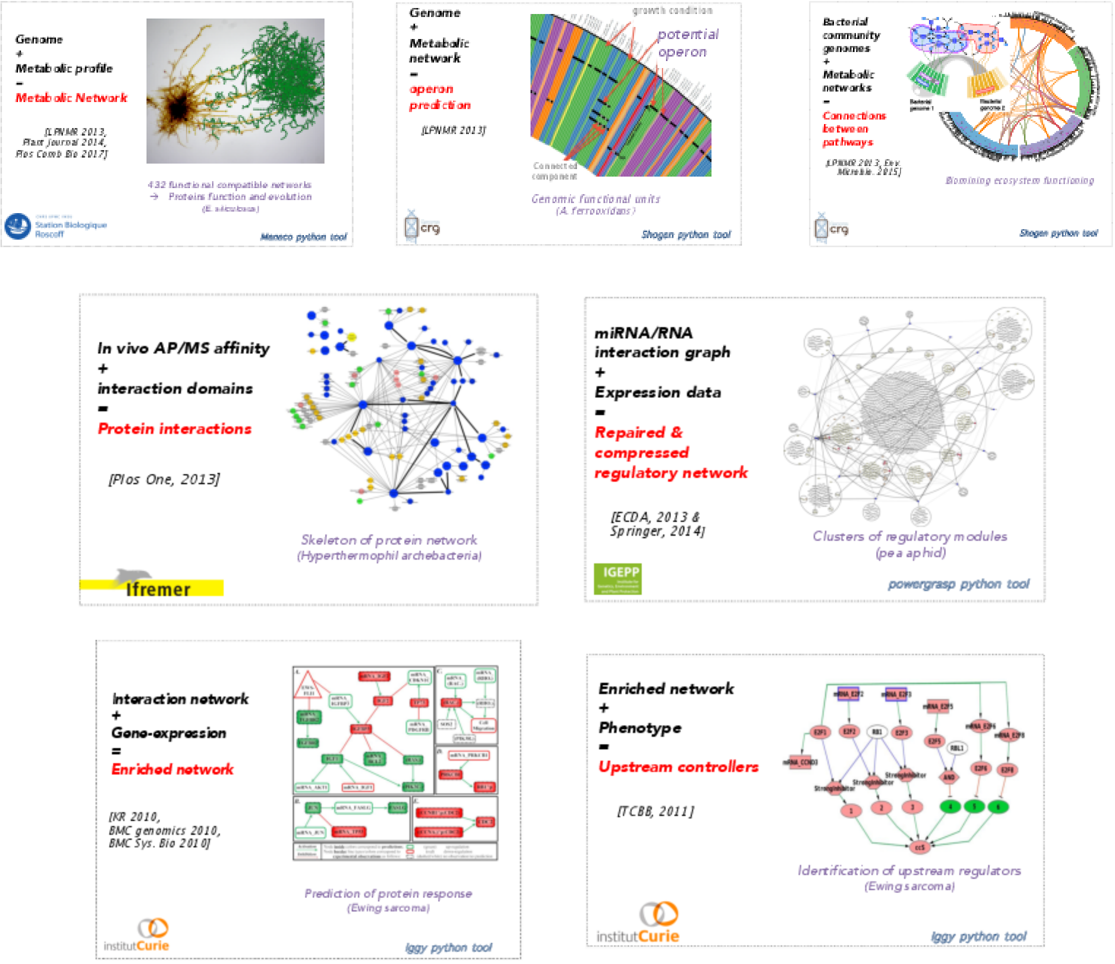
Biological networks are built with data-driven approaches aiming at translating genomic information into a functional map. Most methods are based on a probabilistic framework which defines a probability distribution over the set of models. The reconstructed network is then defined as the most likely model given the data.

Our team has investigated an alternative perspective where each data induces a set of constraints - related to the steady state response of the system dynamics - on the set of possible values in a network of fixed topology. The methods that we have developed complete the network with product states at the level of nodes and influence types at the level of edges, able to globally explain experimental data. In other words, the selection of relevant information in the model is no more performed by selecting *the* network with the highest score, but rather by exploring the complete space of models satisfying constraints on the possible dynamics supported by prior knowledge and observations. In the (common) case when there is no model satisfying all the constraints, we relax the problem by introducing new combinatorial optimization problems that introduce the possibility of correcting the data or the knowledge. Common properties to all solutions are considered as a robust information about the system, as they are independent from the choice of a single solution to the optimization problem [6].

Solving these computational issues requires addressing NP-hard qualitative (non-temporal) issues. We have developed a long-term collaboration with Potsdam University in order to use a logical paradigm named **Answer Set Programming** (ASP) [50], [69] to solve these constraint satisfiability and combinatorial optimization issues. Applied on transcriptomic or cancer networks, our methods identified which regions of a large-scale network shall be corrected [51], and proposed robust corrections [5]. This result suggested that this approach was compatible with efficiency, scale and expressivity needed by biological systems.

During the last years, our goal was to provide **formal models of queries on biological networks** with the focus of integrating dynamical information as explicit logical constraints in the modeling process. Using these technologies requires to revisit and reformulate constraint-satisfiability problems at hand in order both to decrease the search space size in the grounding part of the process and to improve the exploration of this search space in the solving part of the process. Concretely, getting logical encoding for the optimization problems forces to clarify the roles and dependencies between parameters involved in the problem. This paves the way to a refinement approach based on a fine investigation of the space of hypotheses in order to make it smaller and gain in the understanding of the system. Our studies confirmed that logical paradigms are a powerful approach to build and query reconstructed biological systems, in complement to discriminative ("black-box") approaches based on statistical machine-learning. Based on these technologies, we have developed a panel of methods allowing the integration of muli-scale data knowledge, linking genomics, metabolomics, expression data and protein measurement of several phenotypes (see Fig. 1).

Notice that our main issue is in the field of knowledge representation. More precisely, we do not wish to develop new solvers or grounders, a self-contained computational issue which is addressed by specialized teams such as our collaborator team in Potsdam. Our goal is rather to investigate how the constant progresses in the field of constraint logical programming, shown by the performance of ASP-solvers, are sufficient to address the complexity of constraint-satisfiability and combinatorial optimization issues explored in systems biology. In this direction, we work in close interaction with Potsdam university to feed their research activities which challenging issues from bioinformatics and, as a feed-back, take benefit of the prototypes they develop.



Genome
+
Metabolic profile
=
Metabolic Network

[LPNMR 2013,
Plant Journal 2014,
Plos Comb Bio 2017]

432 functional compatible networks
→ Proteins function and evolution
(E. siliculosus)

Station Biologique Roscoff

Meneco python tool

Genome
+
Metabolic network
=
operon prediction

[LPNMR 2013]

Genomic functional units
(A. ferrooxidans)

crg

Shogen python tool

Bacterial community genomes
+
Metabolic networks
=
Connections between pathways

[LPNMR 2013, Env. Microbio. 2015]

Biomining ecosystem functioning

crg

Shogen python tool

In vivo AP/MS affinity
+
interaction domains
=
Protein interactions

[Plos One, 2013]

Skeleton of protein network
(Hyperthermophil archebacteria)

Ifremer

miRNA/RNA interaction graph
+
Expression data
=
Repaired & compressed regulatory network

[ECDA, 2013 &
Springer, 2014]

Clusters of regulatory modules
(pea aphid)

IGEPP

powergrasp python tool

Interaction network
+
Gene-expression
=
Enriched network

[KR 2010,
BMC genomics 2010,
BMC Sys. Bio 2010]

Prediction of protein response
(Ewing sarcoma)

institutCurie

Iggy python tool

Enriched network
+
Phenotype
=
Upstream controllers

[TCBB, 2011]

Identification of upstream regulators
(Ewing sarcoma)

institutCurie

Iggy python tool

*Figure 1. **Multi-scale data and knowledge integration procedures** Dynamical analyses are undergone to elucidate relationships between biological scales. Such dependencies are combined with data and turn into a first order logic paradigm (Answer Set Programming). Key interactions or genes of interest are then identified to be the solution of a combinatorial optimization problem. Methods are encapsulated in python packages and provided in the meta-package bioasp.*

By exploring the complete space of models, our approach typically produces numerous candidate models compatible with the observations. We began investigating to what extent domain knowledge can further refine the analysis of the set of models by identifying classes of similar models, or by selecting a subset of models that satify an additional constraint (for instance, best fit with a set of experiments, or with a minimal size). We anticipate that this will be particularly relevant when studying non-model species for which little is known but valuable information from other species can be transposed or adapted. These efforts consist in developing reasoning methods based on ontologies as formal representation of symbolic knowledge. We use Semantic Web tools such as SPARQL for querying and integrating large sources of external knowledge, and measures of semantic similarity and particularity for analyzing data.

3.2. Modeling the dynamical response of biological systems with logical and (non)-linear constraints

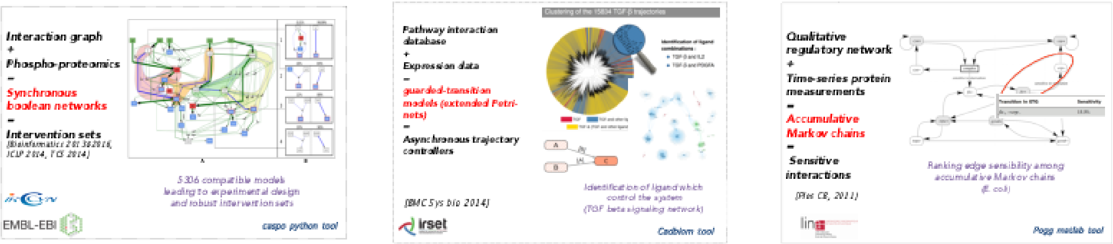
As explained below, Answer Set programming technologies enable the identification of key controllers based on the integration of static data. As a natural follow-up, we also develop optimization techniques to learn models of the dynamics of a biological system. As before, our strategy is not to select a single model fitting with experimental data but rather to decipher the complete set of families of models which a compatible with the observed response. Our main research line in this field is to decipher the appropriate level of expressivity (in terms of constraints) allowing both to properly report the nature of data and knowledge and to allow for an exhaustive study of the space of feasible models. To implement this strategy, we rely on several constraint programming frameworks, which depend on the model scale and the nature of time-points kinetic measurements. The three following examples are shown in Fig. 2 .

- In [7], logical programming (Answer Set programming) is used to decipher the combinatorics ot synchrone boolean networks explaining static or dynamics response of signaling networks to perturbations (such as measured by phosphoproteomics technologies).
- In [49], SAT-based approaches are used to decipher the combinatorics of large-scale asynchronous boolean networks. In order to gain in expressivity, we model these networks as guarded-transition network, an extension of Petri nets.
- In [2] and [47], linear Programming frameworks are used to decipher the variability of the response of reaction-based networks. Still to gain in expressivity, we model systems with Markovian qualitative description of its dynamics together with quantitative laws which describe the effect of the dynamic transitions over higher scale quantitative measurements. Families of models are investigated with ad-hoc local search algorithms.
- Finally, classical learning methods are used to build ad-hoc parameterized numerical models that provide the most parsimonious explanations to experimental measurements.

3.3. Modeling sequences with formal grammars

Once groups of genome products implied in the answer of the species have been identified with integrative or dynamics methods, it remains to characterize the biological actors within genomes. To that goal, we both learn, model and parse formal patterns within DNA, RNA or protein sequences. More precisely, our research on modeling biomolecular sequences with expressive formal grammars focuses on learning such grammars from examples, helping biologists to design their own grammar and providing practical parsing tools.

On the development of **machine learning** algorithms for the induction of grammatical models [40], we have a strong expertise on learning finite state automata. We have proposed an algorithm that learns successfully automata modeling families of (non homologous) functional families of proteins [4], leading to a tool named Protomata-learner (see Fig. 3). The algorthim is based on a similar fragment merging heuristic approach which reports partial and local alignments contained in a family of sequences.. As an example, this tool allowed us to properly model the TNF protein family, a difficult task for classical probabilistic-based approaches. It was also applied successfully to model important enzymatic families of proteins in cyanobacteria [3]. Our future goal is to further demonstrate the relevance of formal language modeling by addressing the question



Interaction graph
+
Phospho-proteomics
=
Synchronous boolean networks
=
Intervention sets
[Bioinformatics 2013, 2016, ICLP 2014, TCS 2014]

5 306 compatible models leading to experimental design and robust intervention sets

caspo python tool

Pathway interaction database
+
Expression data
=
guarded-transition models (extended Petri-nets)
=
Asynchronous trajectory controllers

[BMC Sys bio 2014]

Identification of ligand which control the system (TGF beta signaling network)

Cadbiom tool

Qualitative regulatory network
+
Time-series protein measurements
=
Accumulative Markov chains
=
Sensitive interactions

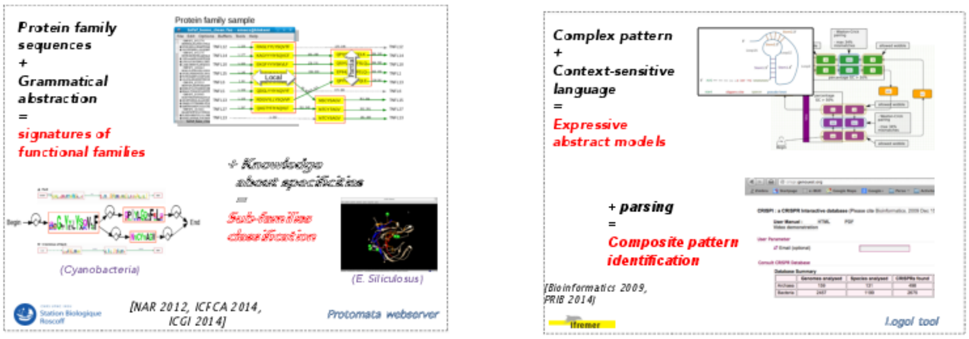
[Plos CB, 2011]

Ranking edge sensibility among accumulative Markov chains (E. coli)

Pogg matlab tool

Figure 2. **Learning and investigating complete families of dynamical models compatible with available data.** *Depending on the scale of the system and the nature of data, we use synchronous boolean networks, enriched Petri Nets or accumulative Markov chains to report and explain the measured response of a biological systems.*

of a fully automatic prediction from the sequence of all the enzymatic families, aiming at improving even more the sensitivity and specificity of the models. As enzyme-substrate interactions are very specific central relations for integrated genome/metabolome studies and are characterized by faint signatures, we shall rely on models for active sites involved in cellular regulation or catalysis mechanisms. This requires to build models gathering both structural and sequence information in order to describe (potentially nested or crossing) long-term dependencies such as contacts of amino-acids that are far in the sequence but close in the 3D protein folding. Our current researches is focused on the inference of Context-Free Grammars including the topological information coming from the structural characterization of active sites.



Protein family sequences
+
Grammatical abstraction
=
signatures of functional families

Protein family sample

+ Knowledge about specificities
=
Sub-families classification

(Cyanobacteria)

(E. Siliculosus)

[NAR 2012, ICFCA 2014, ICGI 2014]

Protomata webserver

Complex pattern
+
Context-sensitive language
=
Expressive abstract models

+ parsing
=
Composite pattern identification

[Bioinformatics 2009, PRIB 2014]

Logol tool

Figure 3. ***Learning and parsing sequences of genome or protein families with expressive grammars**. (a) The protomata workflow starts from a set of protein sequences. A partial local alignment is computed and an automaton is inferred, which can be considered as a signature of the family of proteins. This allows searching for new members of the family [3]. Adding further information about the specific properties of proteins within the family allows to exhibit a refined classification. (b) The Logol framework allows modeling complex structure in sequences, such as a pseudo-knot (RNA structure). This is based on the expressivity of String Variable Grammars. Combined with parsers, this leads to composite pattern identification such as CRISPR. [84].*

Using context-free grammars instead of regular patterns increases the complexity of **parsing** issues. Indeed, efficient parsing tools have been developed to identify patterns within genomes but most of them are restricted to simple regular patterns. Definite Clause Grammars (DCG), a particular form of logical context-free grammars have been used in various works to model DNA sequence features [76]. An extended formalism, String Variable Grammars (SVGs), introduces variables that can be associated to a string during a pattern search (see Fig. 3) [90], [89]. This increases the expressivity of the formalism towards mildly context sensitive grammars. Thus, those grammars model not only DNA/RNA sequence features but also structural features such as repeats, palindromes, stem/loop or pseudo-knots. Few years ago, we have designed a first tool, STAN (suffix-tree analyser), in order to make it possible to search for a subset of SVG patterns in full chromosome sequences [8]. This tool was used for the recognition of transposable elements in *Arabidopsis thaliana* [92]. We have enlarged this experience through a new modeling language, called Logol [1]. Generally, a suitable language for the search of particular components in languages has to meet several needs : expressing existing structures in a compact way, using existing databases of motifs, helping the description of interacting components. In other words, the difficulty is to find a good tradeoff between expressivity and complexity to allow the specification of realistic models at genome scale. The Logol language and associated framework have been built in this direction. See Figure 3 for illustration. The Logol specificity beside other SVG-like languages mainly lies in a systematic introduction of constraints on string variables.

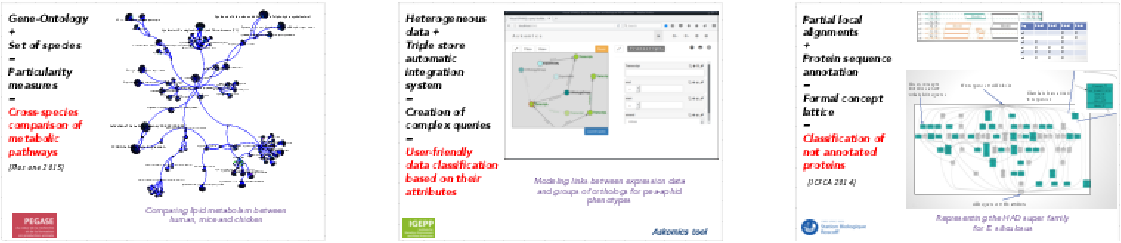
3.4. Symbolic methods for model space exploration: Semantic web for life sciences and Formal Concepts Analysis

All the methods presented in the previous sections usually result in pools of candidates which equivalently explain the data and knowledge. These candidates can be dynamical systems, compounds, biological sequences, proteins... In any case, the output of our formal methods generally requires *a posteriori* investigation and filtering by domain experts. In order to assist them, we rely on two classes of symbolic technics: Semantic Web technologies and Formal Concept Analysis (FCA). They both aim at the formalization and management of knowledge, that is, the explicitation of relations occuring in structured data. These technics complement each other: the production of relevant concepts in FCA highly depends on the availability of semantic annotations using a controlled set of terms and conversely, building and exploiting ontologies is a complex process that can be made much easier with FCA.

Integrating heterogenous data with semantic web technologies The emergence of ontologies in biomedical informatics and bioinformatics happened in parallel with the development of the **Semantic Web** in the computer science community [88]. Let us recall that the Semantic Web is an extension of the current Web that provides an infrastructure integrating data and ontologies in order to support unified reasoning. Since the beginning, life sciences have been a major application domain for the Semantic Web [52]. This was motivated by the joint evolution of data acquisition capabilities in the biomedical field, and of the methods and infrastructures supporting data analysis (grids, the Internet...), resulting in an explosion of data production in complementary domains [60], [53]. Consequently, Semantic Web technologies have become an integral part of translational medicine and translational bioinformatics [63]. The Linked Open Data project promotes the integration of data sources in machine-processable formats compatible with the Semantic Web [59], with a strong involvement of life sciences in this initiative.

However, a specificity of life sciences “data deluge” is that the proportion of generated data is much higher than in the more general “big data phenomenon”, and that these data are highly connected [91]. **The bottleneck that once was data scarcity now lies in the lack of adequate methods supporting data integration, processing and analysis**. [78]. Each of these steps typically hinges on domain knowledge, which is why they resist automation. This knowledge can be seen as the set of rules representing in what conditions data can be used or can be combined for inferring new data or new links between data.

In this setting, we are working on the integration of Semantic Web resources with our data analysis methods in order to take existing biological knowledge into account. We have introduced several methods to interpret semantic similarities and particularities [58], [57]. We now focus our attention on the semi-automated construction of RDF abstractions of heterogeneous datasets which can be handled by non-expert users. This allows both to automatically prepare input datasets for the other methods developed in the team and to analyse the output of the methods in a wide knowledge context.



Gene-Ontology
+
Set of species
–
Particularity measures
–
Cross-species comparison of metabolic pathways
[Bazane 2015]

Comparing lipid metabolism between human, mice and chicken

PEGASE

Heterogeneous data +
Triple store automatic integration system
–
Creation of complex queries
–
User-friendly data classification based on their attributes

Modeling links between expression data and groups of orthologs for pea-aphid phenotypes

IGEPP

Askomics tool

Partial local alignments
+
Protein sequence annotation
–
Formal concept lattice
–
Classification of not annotated proteins
[ICFCA 2014]

Representing the HAD super family for E. siliculosus

Station Biologique Roscoff

Figure 4. ***Data-sciences methods based-on semantic-web technologies and formal concept analysis*** *allows for the knowledge-based post-processing of the results of bioinformatics methods.*

Using Formal concept analysis to explore the results of bioinformatics analyses Formal concept analysis aims at the development of conceptual structures which can be logically activated for the formation of judgments and conclusions [96]. It is used in various domains managing structured data such as knowledge processing, information retrieval or classification [79]. In its most simple form, one considers a binary relation between a set of objects and a set of attributes. In this setting, formal concept analysis formalizes the semantic notions of extension and intension. Concepts are related within a lattice structure (Galois connection) by subconcept-superconcept relations, and this allows drawing causality relations between attribute subsets. In bioinformatics, it has been used to derive phylogenetic relations among groups of organisms [77], a classification task that requires to take into account many-valued Galois connections. We have proposed in a similar way a classification scheme for the problem of protein assignment in a set of protein families [65].

One of the most important issue with concept analysis is due to the fact that current methods remain very sensitive to the presence of uncertainty or incompleteness in data. On the other hand, this apparent defect can be reversed to serve as a marker of incompleteness or inconsistency [66]. Following this inspiration, we have proposed a methodology to tackle the problem of uncertainty on biological networks where edges are mostly predicted links with a high level of false positives [97]. The general idea consists to look for a tradeoff between the simplicity of the conceptual representation and the need to manage exceptions. As a very prospective challenge, we are exploring the idea of using ontologies to help this or to help ontology refinement using concept analysis [80], [56], [83].

More generally, common difficult tasks in this context are visualization, search for local structures (graph mining) and network comparison. Network compression is a good solution for an efficient treatment of all these tasks. This has been used with success in power graphs, which are abstract graphs where nodes are clusters of nodes in the initial graph and edges represent bicliques between two sets of nodes [85]. In fact, concepts are maximal bicliques and we are currently developing the power graph idea in the framework of concept analysis.

ERABLE Project-Team

3. Research Program

3.1. Two main goals

ERABLE has two main goals, one related to biology and the other to methodology (algorithms, combinatorics, statistics). In relation to biology, the main goal of ERABLE is to contribute, through the use of mathematical models and algorithms, to a better understanding of close and often persistent interactions between "collections of genetically identical or distinct self-replicating cells" which will correspond to organisms/species or to actual cells. The first will cover the case of what has been called symbiosis, meaning when the interaction involves different species, while the second will cover the case of a (cancerous) tumour which may be seen as a collection of cells which suddenly disrupts its interaction with the other (collections of) cells in an organism by starting to grow uncontrollably.

Such interactions are being explored initially at the molecular level. Although we rely as much as possible on already available data, we intend to also continue contributing to the identification and analysis of the main genomic and systemic (regulatory, metabolic, signalling) elements involved or impacted by an interaction, and how they are impacted. We started going to the populational and ecological levels by modelling and analysing the way such interactions influence, and are or can be influenced by the ecosystem of which the "collections of cells" are a part. The key steps are:

- identifying the molecular elements based on so-called omics data (genomics, transcriptomics, metabolomics, proteomics, etc.): such elements may be gene/proteins, genetic variations, (DNA/RNA/protein) binding sites, (small and long non coding) RNAs, etc.
- simultaneously inferring and analysing the network that models how these molecular elements are physically and functionally linked together for a given goal, or find themselves associated in a response to some change in the environment;
- modelling and analysing the populational and ecological network formed by the "collections of cells in interaction", meaning modelling a network of networks (previously inferred or as already available in the literature);
- analysing how the behaviour and dynamics of such a network of networks might be controlled by modifying it, including by substracting some of its components from the network or by adding new ones.

In relation to methodology, the main goal is to provide those enabling to address our main biological objective as stated above that lead to the best possible interpretation of the results within a given pre-established model and a well defined question. Ideally, given such a model and question, the method is exact and also exhaustive if more than one answer is possible. Three aspects are thus involved here: establishing the model within which questions can and will be put; clearly defining such questions; exactly answering to them or providing some guarantee on the proximity of the answer given to the "correct" one. We intend to continue contributing to these three aspects:

- at the modelling level, by exploring better models that at a same time are richer in terms of the information they contain (as an example, in the case of metabolism, using hypergraphs as models for it instead of graphs) and are susceptible to an easier treatment:
  - these two objectives (rich models that are at the same time easy to treat) might in many cases be contradictory and our intention is then to contribute to a fuller characterisation of the frontiers between the two;
  - even when feasible, the richer models may lack a full formal characterisation (this is for instance the case of hypergraphs) and our intention is then to contribute to such a characterisation;

- at the question level, by providing clear formalisations of those that will be raised by our biological concerns;
- at the answer level:
  - to extend the area of application of exact algorithms by: (i) a better exploration of the combinatorial properties of the models, (ii) the development of more efficient data structures, (iii) a smarter traversal of the space of solutions when more than one exists;
  - when exact algorithms are not possible, or when there is uncertainty in the input data to an algorithm, to improve the quality of the results given by a deeper exploration of the links between different algorithmic approaches: combinatorial, randomised, stochastic.

3.2. Different research axes

The goals of the team are biological and methodological, the two being intrinsically linked. Any division into axes along one or the other aspect or a combination of both is thus somewhat artificial. Our choice is based more on the biological questions as these are a main (but not unique) driver for the methodological developments. However, since another main objective is to contribute to the fields of exact enumeration algorithms and of combinatorics, we also defined an axis that is exclusively oriented towards some of the more theoretical aspects of such objective in as much as these can be abstracted from the biological motivation. This will concern improving theory and deeply exploring the links between different algorithmic approaches: combinatorial, randomised, stochastic. The first four axes thus fall in the first category, and the fifth one in the second. As concerns the first four axes, the model organisms or systems chosen will be those studied by the biologists among our permanent members or among our close collaborators. Currently these include the following cases:

- Arthropods, notably insects, and their parasites;
- Symbiont-harbouring trypanosomatids and trypanosomas more in general;
- The bacterial communities inside the respiratory tract of mammals (swine, bovine);
- Human in general, and the human microbiota in particular also for its possible relation to cancer.

Notice however that: (1) new model organisms or systems may be considered as the opportunity for new collaborations appears, indeed such collaborations will be actively searched for; and (2) we will always attempt to explore mathematical and computational models and to develop algorithmic methods that are as much as possible generic.

Axis 1: Identifying the molecular elements
Intra and inter-cellular interactions involve molecular elements whose identification is crucial to understand what governs, and also what might enable to control such interactions. For the sake of clarity, the elements may be classified in two main classes, one corresponding to the elements that allow the interactions to happen by moving around or across the cells, and another that are the genomic regions where contact is established. Examples of the first are non coding RNAs, proteins, and mobile genetic elements such as (DNA) transposons, retro-transposons, insertion sequences, etc. Examples of the second are DNA/RNA/protein binding sites and targets. Furthermore, both types (effectors and targets) are subject to variation across individuals of a population, or even within a single (diploid) individual. Identification of these variations is yet another topic that we wish to cover. Variations are understood in the broad sense and cover single nucleotide polymorphisms (SNPs), copy-number variants (CNVs), repeats other than mobile elements, genomic rearrangements (deletions, duplications, insertions, inversions, translocations) and alternative splicings (ASs). All three classes of identification problems (effectors, targets, variations) may be put under the general umbrella of genomic functional annotation.

Axis 2: Inferring and analysing the networks of molecular elements

As increasingly more data about the interaction of molecular elements (among which those described above) becomes available, these should then be modelled in a subsequent step in the form of genetic, metabolic, protein-protein interaction and signalling networks. This raises two main classes of problems. The first is to accurately infer such networks. Reconstructing, by analogy, the metabolic network of an organism is often considered, rightly or wrongly, to be easier than inferring a gene regulatory network, also because in the latter case, identifying all the elements participating in the network is in itself a complex and far from solved issue, as we saw in Axis 1. Moreover, the difficulty varies depending on whether only the structure or also the dynamics of the network is of interest, assuming that the latter may be studied (kinetics data are often missing even with the increasingly more sophisticated and performing technologies we have nowadays). A more complete picture of the functioning of a cell would further require that ever more layers of network and molecular profile data, when available, are integrated together, which raises the problem of how to model together information that is heterogeneous at different levels. Modelling together metabolic and gene regulation for instance is already a hard problem given that the two happen at very different time-scales: fast for metabolic regulation, slow for gene regulation.

Even assuming such a network, integrated or "simple", has been inferred for a given organism or set of organisms, the second problem is then to develop the appropriate mathematical models and methods to extract further biological information from such networks. The difficulty of this differs of course again depending on whether only the structure of the network is of interest, or also its dynamics. We are addressing various questions related to one or the other of the above aspects – inference and analysis.

Axis 3: Modelling and analysing a network of individuals, or a network of individuals' networks

As mentioned, at its extreme, life can be seen as one collection, or a collection of collections of genetically identical or distinct self-replicating cells who interact, sometimes closely and for long periods of evolutionary time, with a same or with distinct functional objectives. One striking example is human, who is composed of cells which are both native and extraneous; in fact, a surprising 90% is believed to belong to the second category, mostly bacteria, including one which lost its identity to become a "mere" human organelle, the mitochondrion. Bacteria on the other hand group into colonies of genetically identical individuals which may sometimes acquire the ability to become specialised for different tasks. Which is the "individual", a single bacterium or a group thereof is difficult to say. To understand human or bacteria, or to understand any other organism, it appears therefore essential to better comprehend the interactions in which they are involved. Methodologically speaking, we must therefore move towards modelling and analysing not a single individual anymore but a network of individuals. Ultimately, we should move towards investigating a network of individuals' networks. Moreover, since organisms interact not only with others but also with their abiotic environment, there is a need to model full ecosystems, at a static but also at a dynamic level, that is by taking into account the fact that individuals or populations move in space. Our intention at a longer term is to address all such different levels. We started with the molecular and static one that we are treating from different perspectives for a large number of species at the genomic level (Baudet *et al.*, Syst Biol, 64(3), 2015) and for a small number at the network level (Cottret *et al.*, PLoS Comput Biol, 6(9), 2010). We intend in a near future to slowly move towards a populational and ecological approach that is dynamic in both time and space.

Axis 4: Going towards control

What was described in the Axes 2 and 3 above concerned modelling and analysing a molecular network, or network of networks, but not attempting to control the network at either level for bio-technological, environmental or health purposes.

In the bio-technological case, the objective can be briefly described as involving the manipulation of a species, in general a bacterium, in order for it to produce more of a given chemical compound it already synthetises (for instance, ethanol) but not in enough quantity, or to produce a metabolite it normally is not able to synthetise. The motivation for transplanting its production in a bacterium is, again, to be able to make it more effective.

As concerns control for environmental or health purposes, this could be achieved at least in some cases by manipulating the symbionts with which an organism, insect pest for instance, or humans leave. In the environmental case, this has gone under the name of “biological control” (see for instance Flint & Dreistat, “Natural Enemies Handbook: The Illustrated Guide to Biological Pest Control”, University of California Press, 1998) and involves the use of “natural enemies” of a pest organism. This idea has a long history: the ancient Chinese, observing that ants were effective predators of many citrus pests, decided to increase the ants population by displacing their nests from the surrounding habitats and placing them inside their orchards to protect them. More recently, there has been growing evidence that some endosymbiotic bacteria, that is bacteria that live within the cells of their hosts, could become efficient biocontrol agents. This is in particular the case of *Wolbachia*, a bacterium much studied in ERABLE (Ahantarig & Kittayapong, J Appl Entomology, 135(7):479-486, 2011).

The connection between disease and the disruption of homeostatic interactions between the host and its microbiota is on the other hand now well established. Microbiota-targeted therapies involve altering the community composition by eliminating individual strains of a single species (for example, with antibiotics) or replacing the entire community with a new intact microbiota. Secondary infections linked to antibiotic use provide however a cautionary tale of the possible consequences of perturbing a microbial species network.

Besides the biotechnological aspects on which we are already working in the context of two European projects (BacHBerry, and to a lesser extent, MicroWine), our main goal in this case is to try to formalise such type of control. There are two objectives here. One is methodological and concerns attempting to provide a single formal framework for the diverse ways of controlling a network, or a network of networks. Our attention has concentrated initially on metabolism, and will at a mid to longer term include regulation. Our intention notably as concerns the incorporation of regulation is to collaborate with other Inria teams, most notably IBIS with whom we are already in discussion. The second objective is biological and concerns control for environmental and health purposes. The originality we are seeking in this case is to attempt such control not by eliminating species, which is done mainly through the use of antibiotics that may then create resistance, a phenomenon that is becoming a major clinical and public health problem, but by manipulating the species or their environment, or by changing the composition of the community by adding or displacing some other species in such a way that new equilibria may be reached which enable all the species living in a same niche to survive. The idea is not new: the areas of prebiotics (non-digestible food ingredients that stimulate the growth and/or activity of bacteria in the digestive system in beneficial ways) and probiotics (micro-organisms claimed to provide benefits when consumed) indeed cover similar concerns in relation to health. Other novel approaches propose to work at the level of bacterial communication (quorum sensing) to control for pathogenicity (Rutherford & Bassler, Cold Spring Harbor Perspectives in Medicine, 2012). Small RNAs in particular are believed to play an important role in quorum sensing.

Axis 5: Cross-fertilising different computational approaches

In computer science and in optimisation, different approaches and techniques have been proposed to cope with hardness results. It is clear that none of them is dominant: there are classes of problems for which approach A is better than approach B, and vice-versa. Moreover, there is no satisfactory understanding of the conditions that favour one approach with respect to another one.

As an example, the team that gave birth to ERABLE, BAMBOO, had expertise more in the area of combinatorial algorithms for strings (sequences), trees and graphs. Many such algorithms addressed an enumeration problem: given a certain description of the object(s) searched for or definition of a function to be optimised, the method was supposed to list all the solutions. In many real life situations, notably in biology, a majority of the problems treated, of whatever kind, enumeration or else, are however hard. Although combinatorics remains crucial to better understand the structure of such problems and delimit the conditions that could render them easy or at least tractable in practice, often other types of approaches have to be attempted.

Although all approaches may be valid and valuable, in many cases one only is explored. More in general, there appears to be relatively little cross-talk and cross-fertilisation being attempted between these different approaches. Guided by problems from computational biology, the goal of this axis is to add to the growing insights on how well such problems can be solved theoretically.

FLUMINANCE Project-Team

3. Research Program

3.1. Estimation of fluid characteristic features from images

The measurement of fluid representative features such as vector fields, potential functions or vorticity maps, enables physicists to have better understanding of experimental or geophysical fluid flows. Such measurements date back to one century and more but became an intensive subject of research since the emergence of correlation techniques [47] to track fluid movements in pairs of images of a particles laden fluid or by the way of clouds photometric pattern identification in meteorological images. In computer vision, the estimation of the projection of the apparent motion of a 3D scene onto the image plane, referred to in the literature as optical-flow, is an intensive subject of researches since the 80's and the seminal work of B. Horn and B. Schunk [57]. Unlike to dense optical flow estimators, the former approach provides techniques that supply only sparse velocity fields. These methods have demonstrated to be robust and to provide accurate measurements for flows seeded with particles. These restrictions and their inherent discrete local nature limit too much their use and prevent any evolutions of these techniques towards the devising of methods supplying physically consistent results and small scale velocity measurements. It does not authorize also the use of scalar images exploited in numerous situations to visualize flows (image showing the diffusion of a scalar such as dye, pollutant, light index refraction, flurocein,...). At the opposite, variational techniques enable in a well-established mathematical framework to estimate spatially continuous velocity fields, which should allow more properly to go towards the measurement of smaller motion scales. As these methods are defined through PDE's systems they allow quite naturally constraints to be included such as kinematic properties or dynamic laws governing the observed fluid flows. Besides, within this framework it is also much easier to define characteristic features estimation procedures on the basis of physically grounded data model that describes the relation linking the observed luminance function and some state variables of the observed flow. The Fluminance group has allowed a substantial progress in this direction with the design of dedicated dense estimation techniques to estimate dense fluid motion fields. See [8] for a detailed review. More recently problems related to scale measurement and uncertainty estimation have been investigated [51]. Dynamically consistent and highly robust techniques have been also proposed for the recovery of surface oceanic streams from satellite images [49].

3.2. Data assimilation and Tracking of characteristic fluid features

Real flows have an extent of complexity, even in carefully controlled experimental conditions, which prevents any set of sensors from providing enough information to describe them completely. Even with the highest levels of accuracy, space-time coverage and grid refinement, there will always remain at least a lack of resolution and some missing input about the actual boundary conditions. This is obviously true for the complex flows encountered in industrial and natural conditions, but remains also an obstacle even for standard academic flows thoroughly investigated in research conditions.

This unavoidable deficiency of the experimental techniques is nevertheless more and more compensated by numerical simulations. The parallel advances in sensors, acquisition, treatment and computer efficiency allow the mixing of experimental and simulated data produced at compatible scales in space and time. The inclusion of dynamical models as constraints of the data analysis process brings a guaranty of coherency based on fundamental equations known to correctly represent the dynamics of the flow (e.g. Navier Stokes equations) [11]. Conversely, the injection of experimental data into simulations ensures some fitting of the model with reality.

To enable data and models coupling to achieve its potential, some difficulties have to be tackled. It is in particular important to outline the fact that the coupling of dynamical models and image data are far from being straightforward. The first difficulty is related to the space of the physical model. As a matter of fact, physical models describe generally the phenomenon evolution in a 3D Cartesian space whereas images provides generally only 2D tomographic views or projections of the 3D space on the 2D image plane. Furthermore, these views are sometimes incomplete because of partial occlusions and the relations between the model state variables and the image intensity function are otherwise often intricate and only partially known. Besides, the dynamical model and the image data may be related to spatio-temporal scale spaces of very different natures which increases the complexity of an eventual multiscale coupling. As a consequence of these difficulties, it is necessary generally to define simpler dynamical models in order to assimilate image data. This redefinition can be done for instance on an uncertainty analysis basis, through physical considerations or by the way of data based empirical specifications. Such modeling comes to define inexact evolution laws and leads to the handling of stochastic dynamical models. The necessity to make use and define sound approximate models, the dimension of the state variables of interest and the complex relations linking the state variables and the intensity function, together with the potential applications described earlier constitute very stimulating issues for the design of efficient data-model coupling techniques based on image sequences.

On top of the problems mentioned above, the models exploited in assimilation techniques often suffer from some uncertainties on the parameters which define them. Hence, a new emerging field of research focuses on the characterization of the set of achievable solutions as a function of these uncertainties. This sort of characterization indeed turns out to be crucial for the relevant analysis of any simulation outputs or the correct interpretation of operational forecasting schemes. In this context, the tools provided by the Bayesian theory play a crucial role since they encompass a variety of methodologies to model and process uncertainty. As a consequence, the Bayesian paradigm has already been present in many contributions of the Fluminance group in the last years and will remain a cornerstone of the new methodologies investigated by the team in the domain of uncertainty characterization.

This wide theme of research problems is a central topic in our research group. As a matter of fact, such a coupling may rely on adequate instantaneous motion descriptors extracted with the help of the techniques studied in the first research axis of the FLUMINANCE group. In the same time, this coupling is also essential with respect to visual flow control studies explored in the third theme. The coupling between a dynamics and data, designated in the literature as a Data Assimilation issue, can be either conducted with optimal control techniques [58], [59] or through stochastic filtering approaches [52], [55]. These two frameworks have their own advantages and deficiencies. We rely indifferently on both approaches.

3.3. Optimization and control of fluid flows with visual servoing

Fluid flow control is a recent and active research domain. A significant part of the work carried out so far in that field has been dedicated to the control of the transition from laminarity to turbulence. Delaying, accelerating or modifying this transition is of great economical interest for industrial applications. For instance, it has been shown that for an aircraft, a drag reduction can be obtained while enhancing the lift, leading consequently to limit fuel consumption. In contrast, in other application domains such as industrial chemistry, turbulence phenomena are encouraged to improve heat exchange, increase the mixing of chemical components and enhance chemical reactions. Similarly, in military and civilians applications where combustion is involved, the control of mixing by means of turbulence handling rouses a great interest, for example to limit infra-red signatures of fighter aircraft.

Flow control can be achieved in two different ways: passive or active control. Passive control provides a permanent action on a system. Most often it consists in optimizing shapes or in choosing suitable surfacing (see for example [50] where longitudinal riblets are used to reduce the drag caused by turbulence). The main problem with such an approach is that the control is, of course, inoperative when the system changes. Conversely, in active control the action is time varying and adapted to the current system's state. This approach requires an external energy to act on the system through actuators enabling a forcing on the flow through for instance blowing and suction actions [62], [54]. A closed-loop problem can be formulated as an optimal control issue where a control law minimizing an objective cost function (minimization of the drag, minimization of the actuators power, etc.) must be applied to the actuators [48]. Most of the works of the literature indeed comes back to open-loop control approaches [61], [56], [60] or to forcing approaches [53] with control laws acting without any feedback information on the flow actual state. In order for these methods to be operative, the model used to derive the control law must describe as accurately as possible the flow and all the eventual perturbations of the surrounding environment, which is very unlikely in real situations. In addition, as such approaches rely on a perfect model, a high computational costs is usually required. This inescapable pitfall has motivated a strong interest on model reduction. Their key advantage being that they can be specified empirically from the data and represent quite accurately, with only few modes, complex flows' dynamics. This motivates an important research axis in the Fluminance group.

3.4. Numerical models applied to hydrogeology and geophysics

The team is strongly involved in numerical models for hydrogeology and geophysics. There are many scientific challenges in the area of groundwater simulations. This interdisciplinary research is very fruitful with cross-fertilizing subjects. For example, high performance simulations were very helpful for finding out the asymptotic behaviour of the plume of solute transported by advection-dispersion. Numerical models are necessary to understand flow transfer in fractured media.

The team develops stochastic models for groundware simulations as well as for oceanic and atmospheric flows. Numerical models must then include Uncertainty Quantification methods, spatial and time discretization. Then, the discrete problems must be solved with efficient algorithms. The team develops parallel algorithms for complex numerical simulations and conducts performance analysis.

3.5. Numerical algorithms and high performance computing

Linear algebra is at the kernel of most scientific applications, in particular in physical or chemical engineering. For example, steady-state flow simulations in porous media are discretized in space and lead to a large sparse linear system. The target size is 10^7 in 2D and 10^{10} in 3D. For transient models such as diffusion, the objective is to solve about 10^4 linear systems for each simulation. Memory requirements are of the order of Giga-bytes in 2D and Tera-bytes in 3D. CPU times are of the order of several hours to several days. Several methods and solvers exist for large sparse linear systems. They can be divided into three classes: direct, iterative or semi-iterative. Direct methods are highly efficient but require a large memory space and a rapidly increasing computational time. Iterative methods of Krylov type require less memory but need a scalable preconditioner to remain competitive. Iterative methods of multigrid type are efficient and scalable, used by themselves or as preconditioners, with a linear complexity for elliptic or parabolic problems but they are not so efficient for hyperbolic problems. Semi-iterative methods such as subdomain methods are hybrid direct/iterative methods which can be good tradeoffs. The convergence of iterative and semi-iterative methods and the accuracy of the results depend on the condition number which can blow up at large scale. The objectives are to analyze the complexity of these different methods, to accelerate convergence of iterative methods, to measure and improve the efficiency on parallel architectures, to define criteria of choice.

In geophysics, a main concern is to solve inverse problems in order to fit the measured data with the model. Generally, this amounts to solve a linear or nonlinear least-squares problem. Complex models are in general coupled multi-physics models. For example, reactive transport couples advection-diffusion with chemistry. Here, the mathematical model is a set of nonlinear Partial Differential Algebraic Equations. At each timestep of an implicit scheme, a large nonlinear system of equations arise. The challenge is to solve efficiently and accurately these large nonlinear systems.

Approximation in Krylov subspace is in the core of the team activity since it provides efficient iterative solvers for linear systems and eigenvalue problems as well. The later are encountered in many fields and they include the singular value problem which is especially useful when solving ill posed inverse problems.

GALEN Project-Team

3. Research Program

3.1. Shape, Grouping and Recognition

A general framework for the fundamental problems of image segmentation, object recognition and scene analysis is the interpretation of an image in terms of a set of symbols and relations among them. Abstractly stated, image interpretation amounts to mapping an observed image, X to a set of symbols Y. Of particular interest are the symbols Y^* that *optimally explain the underlying image*, as measured by a scoring function s that aims at distinguishing correct (consistent with human labellings) from incorrect interpretations:

$$Y^* = \mathrm{argmax}_Y s(X, Y) \tag{73}$$

Applying this framework requires (a) identifying which symbols and relations to use (b) learning a scoring function s from training data and (c) optimizing over Y in Eq.1 .

One of the main themes of our work is the development of methods that jointly address (a,b,c) in a shape-grouping framework in order to reliably extract, describe, model and detect shape information from natural and medical images. A principal motivation for using a shape-based framework is the understanding that shape- and more generally, grouping- based representations can go all the way from image features to objects. Regarding aspect (a), image representation, we cater for the extraction of image features that respect the shape properties of image structures. Such features are typically constructed to be purely geometric (e.g. boundaries, symmetry axes, image segments), or appearance-based, such as image descriptors. The use of machine learning has been shown to facilitate the robust and efficient extraction of such features, while the grouping of local evidence is known to be necessary to disambiguate the potentially noisy local measurements. In our research we have worked on improving feature extraction, proposing novel blends of invariant geometric- and appearance- based features, as well as grouping algorithms that allow for the efficient construction of optimal assemblies of local features.

Regarding aspect (b) we have worked on learning scoring functions for detection with deformable models that can exploit the developed low-level representations, while also being amenable to efficient optimization. Our works in this direction build on the graph-based framework to construct models that reflect the shape properties of the structure being modeled. We have used discriminative learning to exploit boundary- and symmetry-based representations for the construction of hierarchical models for shape detection, while for medical images we have developed methods for the end-to-end discriminative training of deformable contour models that combine low-level descriptors with contour-based organ boundary representations.

Regarding aspect (c) we have developed algorithms which implement top-down/bottom-up computation both in deterministic and stochastic optimization. The main idea is that 'bottom-up', image-based guidance is necessary for efficient detection, while 'top-down', object-based knowledge can disambiguate and help reliably interpret a given image; a combination of both modes of operation is necessary to combine accuracy with efficiency. In particular we have developed novel techniques for object detection that employ combinatorial optimization tools (A* and Branch-and-Bound) to tame the combinatorial complexity, achieving a best-case performance that is logarithmic in the number of pixels.

In the long run we aim at scaling up shape-based methods to 3D detection and pose estimation and large-scale object detection. One aspect which seems central to this is the development of appropriate mid-level representations. This is a problem that has received increased interest lately in the 2D case and is relatively mature, but in 3D it has been pursued primarily through ad-hoc schemes. We anticipate that questions pertaining to part sharing in 3D will be addressed most successfully by relying on explicit 3D representations. On the one hand depth sensors, such as Microsoft's Kinect, are now cheap enough to bring surface modeling and matching into the mainstream of computer vision - so these advances may be directly exploitable at test time for detection. On the other hand, even if we do not use depth information at test time, having 3D information can simplify the modeling task during training. In on-going work with collaborators we have started exploring combinations of such aspects, namely (i) the use of surface analysis tools to match surfaces from depth sensors (ii) using branch-and-bound for efficient inference in 3D space and (iii) groupwise-registration to build statistical 3D surface models. In the coming years we intend to pursue a tighter integration of these different directions for scalable 3D object recognition.

3.2. Machine Learning & Structured Prediction

The foundation of statistical inference is to learn a function that minimizes the expected loss of a prediction with respect to some unknown distribution

$$\mathcal{R}(f) = \int \ell(f, x, y) dP(x, y), \tag{74}$$

where $\ell(f, x, y)$ is a problem specific loss function that encodes a penalty for predicting $f(x)$ when the correct prediction is y. In our case, we consider x to be a medical image, and y to be some prediction, e.g. the segmentation of a tumor, or a kinematic model of the skeleton. The loss function, ℓ, is informed by the costs associated with making a specific misprediction. As a concrete example, if the true spatial extent of a tumor is encoded in y, $f(x)$ may make mistakes in classifying healthy tissue as a tumor, and mistakes in classifying diseased tissue as healthy. The loss function should encode the potential physiological damage resulting from erroneously targeting healthy tissue for irradiation, as well as the risk from missing a portion of the tumor.

A key problem is that the distribution P is unknown, and any algorithm that is to estimate f from labeled training examples must additionally make an implicit estimate of P. A central technology of empirical inference is to approximate $\mathcal{R}(f)$ with the empirical risk,

$$\mathcal{R}(f) \approx \widehat{\mathcal{R}}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(f, x_i, y_i), \tag{75}$$

which makes an implicit assumption that the training samples (x_i, y_i) are drawn i.i.d. from P. Direct minimization of $\widehat{\mathcal{R}}(f)$ leads to overfitting when the function class $f \in \mathcal{F}$ is too rich, and regularization is required:

$$\min_{f \in \mathcal{F}} \lambda \Omega(\|f\|) + \widehat{\mathcal{R}}(f), \tag{76}$$

where Ω is a monotonically increasing function that penalizes complex functions.

Equation Eq. 4 is very well studied in classical statistics for the case that the output, $y \in \mathcal{Y}$, is a binary or scalar prediction, but this is not the case in most medical imaging prediction tasks of interest. Instead, complex interdependencies in the output space leads to difficulties in modeling inference as a binary prediction problem. One may attempt to model e.g. tumor segmentation as a series of binary predictions at each voxel in a medical image, but this violates the i.i.d. sampling assumption implicit in Equation Eq. 3 . Furthermore, we typically gain performance by appropriately modeling the inter-relationships between voxel predictions, e.g. by incorporating pairwise and higher order potentials that encode prior knowledge about the problem domain. It is in this context that we develop statistical methods appropriate to structured prediction in the medical imaging setting.

3.3. Self-Paced Learning with Missing Information

Many tasks in artificial intelligence are solved by building a model whose parameters encode the prior domain knowledge and the likelihood of the observed data. In order to use such models in practice, we need to estimate its parameters automatically using training data. The most prevalent paradigm of parameter estimation is supervised learning, which requires the collection of the inputs x_i and the desired outputs y_i. However, such an approach has two main disadvantages. First, obtaining the ground-truth annotation of high-level applications, such as a tight bounding box around all the objects present in an image, is often expensive. This prohibits the use of a large training dataset, which is essential for learning the existing complex models. Second, in many applications, particularly in the field of medical image analysis, obtaining the ground-truth annotation may not be feasible. For example, even the experts may disagree on the correct segmentation of a microscopical image due to the similarities between the appearance of the foreground and background.

In order to address the deficiencies of supervised learning, researchers have started to focus on the problem of parameter estimation with data that contains hidden variables. The hidden variables model the missing information in the annotations. Obtaining such data is practically more feasible: image-level labels ('contains car','does not contain person') instead of tight bounding boxes; partial segmentation of medical images. Formally, the parameters **w** of the model are learned by minimizing the following objective:

$$\min_{\mathbf{w}\in\mathcal{W}} R(\mathbf{w}) + \sum_{i=1}^{n} \Delta(y_i, y_i(\mathbf{w}), h_i(\mathbf{w})). \tag{77}$$

Here, $\mathcal{W}$ represents the space of all parameters, n is the number of training samples, $R(\cdot)$ is a regularization function, and $\Delta(\cdot)$ is a measure of the difference between the ground-truth output y_i and the predicted output and hidden variable pair $(y_i(\mathbf{w}), h_i(\mathbf{w}))$.

Previous attempts at minimizing the above objective function treat all the training samples equally. This is in stark contrast to how a child learns: first focus on easy samples ('learn to add two natural numbers') before moving on to more complex samples ('learn to add two complex numbers'). In our work, we capture this intuition using a novel, iterative algorithm called self-paced learning (SPL). At an iteration t, SPL minimizes the following objective function:

$$\min_{\mathbf{w}\in\mathcal{W},\mathbf{v}\in\{0,1\}^n} R(\mathbf{w}) + \sum_{i=1}^{n} v_i \Delta(y_i, y_i(\mathbf{w}), h_i(\mathbf{w})) - \mu_t \sum_{i=1}^{n} v_i. \tag{78}$$

Here, samples with $v_i = 0$ are discarded during the iteration t, since the corresponding loss is multiplied by 0. The term μ_t is a threshold that governs how many samples are discarded. It is annealed at each iteration, allowing the learner to estimate the parameters using more and more samples, until all samples are used. Our results already demonstrate that SPL estimates accurate parameters for various applications such as image classification, discriminative motif finding, handwritten digit recognition and semantic segmentation. We will investigate the use of SPL to estimate the parameters of the models of medical imaging applications, such as segmentation and registration, that are being developed in the GALEN team. The ability to handle missing information is extremely important in this domain due to the similarities between foreground and background appearances (which results in ambiguities in annotations). We will also develop methods that are capable of minimizing more general loss functions that depend on the (unknown) value of the hidden variables, that is,

$$\min_{\mathbf{w}\in\mathcal{W},\theta\in\Theta} R(\mathbf{w}) + \sum_{i=1}^{n} \sum_{h_i\in\mathcal{H}} \Pr(h_i|x_i, y_i; \theta) \Delta(y_i, h_i, y_i(\mathbf{w}), h_i(\mathbf{w})). \tag{79}$$

Here, θ is the parameter vector of the distribution of the hidden variables h_i given the input x_i and output y_i, and needs to be estimated together with the model parameters $\mathbf{w}$. The use of a more general loss function will allow us to better exploit the freely available data with missing information. For example, consider the case where y_i is a binary indicator for the presence of a type of cell in a microscopical image, and h_i is a tight bounding box around the cell. While the loss function $\Delta(y_i, y_i(\mathbf{w}), h_i(\mathbf{w}))$ can be used to learn to classify an image as containing a particular cell or not, the more general loss function $\Delta(y_i, h_i, y_i(\mathbf{w}), h_i(\mathbf{w}))$ can be used to learn to detect the cell as well (since h_i models its location)

3.4. Discrete Biomedical Image Perception

A wide variety of tasks in medical image analysis can be formulated as discrete labeling problems. In very simple terms, a discrete optimization problem can be stated as follows: we are given a discrete set of variables $\mathcal{V}$, all of which are vertices in a graph $\mathcal{G}$. The edges of this graph (denoted by $\mathcal{E}$) encode the variables' relationships. We are also given as input a discrete set of labels $\mathcal{L}$. We must then assign one label from $\mathcal{L}$ to each variable in $\mathcal{V}$. However, each time we choose to assign a label, say, x_{p_1} to a variable p_1, we are forced to pay a price according to the so-called *singleton* potential function $g_p(x_p)$, while each time we choose to assign a pair of labels, say, x_{p_1} and x_{p_2} to two interrelated variables p_1 and p_2 (two nodes that are connected by an edge in the graph $\mathcal{G}$), we are also forced to pay another price, which is now determined by the so called *pairwise* potential function $f_{p_1p_2}(x_{p_1}, x_{p_2})$. Both the singleton and pairwise potential functions are problem specific and are thus assumed to be provided as input.

Our goal is then to choose a labeling which will allow us to pay the smallest total price. In other words, based on what we have mentioned above, we want to choose a labeling that minimizes the sum of all the MRF potentials, or equivalently the MRF energy. This amounts to solving the following optimization problem:

$$\arg\min_{\{x_p\}} \mathcal{P}(g, f) = \sum_{p \in \mathcal{V}} g_p(x_p) + \sum_{(p_1, p_2) \in \mathcal{E}} f_{p_1p_2}(x_{p_1}, x_{p_2}). \tag{80}$$

The use of such a model can describe a number of challenging problems in medical image analysis. However these simplistic models can only account for simple interactions between variables, a rather constrained scenario for high-level medical imaging perception tasks. One can augment the expression power of this model through higher order interactions between variables, or a number of cliques $\{C_i, i \in [1, n] = \{\{p_{i^1}, \cdots, p_{i^{|C_i|}}\}\}$ of order $|C_i|$ that will augment the definition of $\mathcal{V}$ and will introduce hyper-vertices:

$$\arg\min_{\{x_p\}} \mathcal{P}(g, f) = \sum_{p \in \mathcal{V}} g_p(x_p) + \sum_{(p_1, p_2) \in \mathcal{E}} f_{p_1p_2}(x_{p_1}, x_{p_2}) + \sum_{C_i \in \mathcal{E}} f_{p_1 \cdots p_n}(x_{p_{i^1}}, \cdots, p_{x_{i^{|C_i|}}}). \tag{81}$$

where $f_{p_1 \cdots p_n}$ is the price to pay for associating the labels $(x_{p_{i^1}}, \cdots, p_{x_{i^{|C_i|}}})$ to the nodes $(p_1 \cdots p_{i^{|C_i|}})$. Parameter inference, addressed by minimizing the problem above, is the most critical aspect in computational medicine and efficient optimization algorithms are to be evaluated both in terms of computational complexity as well as of inference performance. State of the art methods include deterministic and non-deterministic annealing, genetic algorithms, max-flow/min-cut techniques and relaxation. These methods offer certain strengths while exhibiting certain limitations, mostly related to the amount of interactions which can be tolerated among neighborhood nodes. In the area of medical imaging where domain knowledge is quite strong, one would expect that such interactions should be enforced at the largest scale possible.

GENSCALE Project-Team

3. Research Program

3.1. Introduction

Based on these overall objectives, the research program of GenScale is structured into four research axes as described below. The first three axes include pure computer science aspects, such as the development of advanced data structures and/or the design of new optimized algorithms; they also include strong partnerships with life science actors to validate the methodologies that are developed. The fourth axis can be seen as a transversal one. It addresses efficient parallel implementations of our methods on standard processors, cluster systems, or accelerators such as GPU.

3.2. Axis 1: HTS data processing

The raw information delivered by NGS (Next Generation Sequencing) technologies represents billions of short DNA fragments. An efficient structuration of this mass of data is the de-Bruijn graph that is used for a large panel of problems dealing with high throughput genomic data processing. The challenge, here, is to represent this graph into memory. An efficient way is to use probabilistic data structures, such as Bloom filters but they generate false positives that introduce noise and may lead to errors. Our approach is to enhance this basic data structure with extra information to provide exact answers, while keeping a minimal memory occupancy [3], [4].

Based on this central data structure, a large panel of HTS algorithms can be designed: read compression, read correction, genome assembly, detection of SNPs (Single Nucleotide Polymorphism) or detection of other variants such as inversion, transposition, etc [10], [8]. The use of this compact structure guarantees software with very low memory footprint that can be executed on many standard-computing resources.

In the full assembly process, an open problem due to the structure complexity of many genomes is the scaffolding step that consists in reordering contigs along the chromosomes. This treatment can be formulated as a combinatorial optimization problem exploiting the upcoming new sequencing technologies based on long reads.

3.3. Axis 2: Sequence comparison

Comparing genomic sequences (DNA, RNA, protein) is a basic bioinformatics task. Powerful heuristics (such as the seed-extend heuristic used in the well-known BLAST software) have been proposed to limit the computation time. The underlying data structures are based on seed indexes allowing a drastic reduction of the search space. However, due to the increasing flux of genomic sequences, this treatment tends to increase and becomes a critical section, especially in metagenomic projects where hundred of millions of reads must be compared to large genomic banks for taxonomic of functional assignation.

Our research follows mainly two directions. The first one revisits the seed-extend heuristic in the context of the bank-to-bank comparison problem. It requires new data structures to better classify the genomic information, and new algorithmic methods to navigate through this mass of data [7], [9]. The second one addresses metagenomic challenges that have to extract relevant knowledge from Tera bytes of data. In that case, the notion of sequence similarity itself is redefined in order to work on objects that are much simpler than the standard alignment score, and that are better suited for large-scale computation. Raw information (reads) is first reduced to k-mers from which high speed and parallel algorithms compute approximate similarities based on a well defined statistical model [5], [2].

3.4. Axis 3: Protein 3D structure

The three-dimensional (3D) structure of proteins tends to be evolutionarily better preserved during evolution than its sequence. Finding structural similarities between proteins gives deep insights into whether these proteins share a common function or whether they are evolutionarily related. Structural similarity between two proteins is usually defined by two functions – a one to- one mapping (also called alignment) between two subchains of their 3D representations and a specific scoring function that assesses the alignment quality. The structural alignment problem is to find the mapping that is optimal with respect to the scoring function. Protein structures can be represented as graphs, and the problem reduces to various combinatorial optimization problems that can be formulated in this framework: for example finding the maximum weighted path [1] or finding the maximum cardinality clique/pseudo-clique [6].

In most cases, however, suitable conformations for a given protein are unknown. To support this statement, we point out that the number of deposited protein conformations on the Protein Data Bank (PDB [0]) recently reached the threshold of 110,000 entries, while the UniProtKB/TrEMBL [0] database contains more than 50 million sequence entries, all of them potentially capable for coding for a new protein. In this context, distance geometry provides powerful methods and algorithms for the identification of protein conformations from Nuclear Magnetic Resonance (NMR) data, which basically consist of a distance list concerning atom pairs of the protein. We are working on the discretization of the distance geometry, so that its search space becomes discrete (and finite!), for making it possible to perform an exhaustive exploration of the solution set.

3.5. Axis 4: Parallelism

Together with the design of new data structures and new algorithms, our research program aims to propose efficient hardware implementation. Even if not explicitly mentioned in the three previous axes, we have constantly in mind to exploit the parallelism of current processors. Practically, and depending on the nature of the computation to perform, three levels of parallelism are addressed: the use of vector instructions of today processors, the multithreading offered by multi-core systems, and the cluster (or cloud) infrastructures.

Consequent bioinformatics treatments, from the processing of raw HTS data to high-level analysis, are generally performed within a workflow environment and executed on cluster systems. Automating the parallelization of such treatments directly from a graphical capture of the workflow is a necessity for end-users that are generally not expert in parallelism. The challenge here is to hide, as much as possible, the different transformations to go from a high level workflow description to an efficient parallel execution that exploits both task-level and data-level parallelism.

Another research activity of this axe is the design of parallel algorithms targeting hardware accelerators, especially GPU boards (Graphical Processing Unit). These devices now offer a high-level programming environment to access the hundred of processors available on a single chip. A few bioinformatics treatments, such as the ones that exhibit good computational regularity, can highly benefit from the computing power of this technology.

[0] http://www.rcsb.org/
[0] http://www.ebi.ac.uk/uniprot/TrEMBLstats

IBIS Project-Team

3. Research Program

3.1. Analysis of qualitative dynamics of gene regulatory networks

Participants: Hidde de Jong [Correspondent], Michel Page.

The dynamics of gene regulatory networks can be modeled by means of ordinary differential equations (ODEs), describing the rate of synthesis and degradation of the gene products as well as regulatory interactions between gene products and metabolites. In practice, such models are not easy to construct though, as the parameters are often only constrained to within a range spanning several orders of magnitude for most systems of biological interest. Moreover, the models usually consist of a large number of variables, are strongly nonlinear, and include different time-scales, which makes them difficult to handle both mathematically and computationally. This has motivated the interest in qualitative models which, from incomplete knowledge of the system, are able to provide a coarse-grained picture of its dynamics.

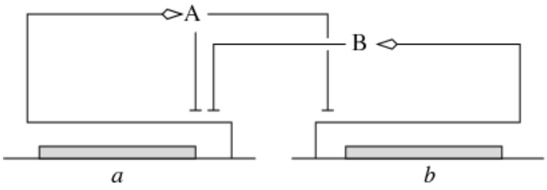
A variety of qualitative modeling formalisms have been introduced over the past decades. Boolean or logical models, which describe gene regulatory and signalling networks as discrete-time finite-state transition systems, are probably most widely used. The dynamics of these systems are governed by logical functions representing the regulatory interactions between the genes and other components of the system. IBIS has focused on a related, hybrid formalism that embeds the logical functions describing regulatory interactions into an ODE formalism, giving rise to so-called piecewise-linear differential equations (PLDEs, Figure 2). The use of logical functions allows the qualitative dynamics of the PLDE models to be analyzed, even in high-dimensional systems. In particular, the qualitative dynamics can be represented by means of a so-called state transition graph, where the states correspond to (hyperrectangular) regions in the state space and transitions between states arise from solutions entering one region from another.

First proposed by Leon Glass and Stuart Kauffman in the early seventies, the mathematical analysis of PLDE models has been the subject of active research for more than four decades. IBIS has made contributions on the mathematical level, in collaboration with the BIOCORE and BIPOP project-teams, notably for solving problems induced by discontinuities in the dynamics of the system at the boundaries between regions, where the logical functions may abruptly switch from one discrete value to another, corresponding to the (in)activation of a gene. In addition, many efforts have gone into the development of the computer tool GENETIC NETWORK ANALYZER (GNA) and its applications to the analysis of the qualitative dynamics of a variety of regulatory networks in microorganisms. Some of the methodological work underlying GNA, notably the development of analysis tools based on temporal logics and model checking, which was carried out with the Inria project-teams CONVEX (ex-VASY) and POP-ART, has implications beyond PLDE models as they apply to logical and other qualitative models as well.

3.2. Inference of gene regulatory networks from time-series data

Participants: Eugenio Cinquemani [Correspondent], Johannes Geiselmann, Hidde de Jong, Cyril Dutrieux, Stephan Lacour, Yannick Martin, Michel Page, Corinne Pinel, Delphine Ropers.

Measurements of the transcriptome of a bacterial cell by means of DNA microarrays, RNA sequencing, and other technologies have yielded huge amounts of data on the state of the transcriptional program in different growth conditions and genetic backgrounds, across different time-points in an experiment. The information on the time-varying state of the cell thus obtained has fueled the development of methods for inferring regulatory interactions between genes. In essence, these methods try to explain the observed variation in the activity of one gene in terms of the variation in activity of other genes. A large number of inference methods have been proposed in the literature and have been successful in a variety of applications, although a number of difficult problems remain.



$$\dot{x}_a = \kappa_a \, s^-(x_a, \theta_a^2) \, s^-(x_b, \theta_b) - \gamma_a \, x_a$$

$$\dot{x}_b = \kappa_b \, s^-(x_a, \theta_a^1) - \gamma_b \, x_b$$

$$s^+(x, \theta) = \begin{cases} 1, & \text{if } x > \theta \\ 0, & \text{if } x < \theta \end{cases}$$

$$s^-(x, \theta) = 1 - s^+(x, \theta)$$

Figure 2. (Left) Example of a gene regulatory network of two genes (a and b), each coding for a regulatory protein (A and B). Protein B inhibits the expression of gene a, while protein A inhibits the expression of gene b and its own gene. (Right) PLDE model corresponding to the network in (a). Protein A is synthesized at a rate κ_a, if and only if the concentration of protein A is below its threshold θ_a^2 ($x_a < \theta_a^2$) and the concentration of protein B below its threshold θ_b ($x_b < \theta_b$). The degradation of protein A occurs at a rate proportional to the concentration of the protein itself ($\gamma_a \, x_a$).

Current reporter gene technologies, based on Green Fluorescent Proteins (GFPs) and other fluorescent and luminescent reporter proteins, provide an excellent means to measure the activity of a gene *in vivo* and in real time (Figure 3). The underlying principle of the technology is to fuse the promoter region and possibly (part of) the coding region of a gene of interest to a reporter gene. The expression of the reporter gene generates a visible signal (fluorescence or luminescence) that is easy to capture and reflects the expression of a gene of interest. The interest of the reporter systems is further enhanced when they are applied in mutant strains or combined with expression vectors that allow the controlled induction of any particular gene, or the degradation of its product, at a precise moment during the time-course of the experiment. This makes it possible to perturb the network dynamics in a variety of ways, thus obtaining precious information for network inference.

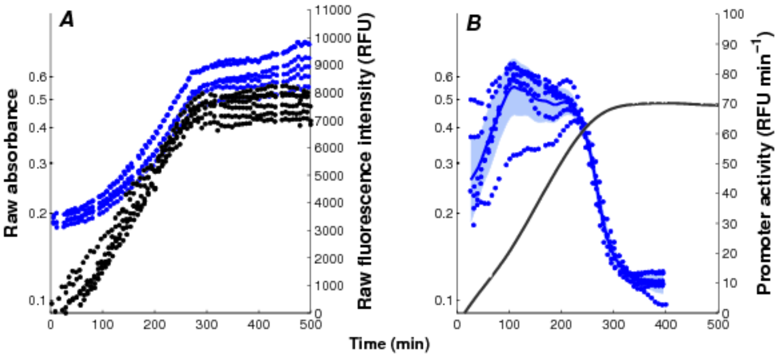


Figure 3. Monitoring of bacterial gene expression in vivo using fluorescent reporter genes (Stefan et al., PLoS Computational Biology, 11(1):e1004028, 2015). The plots show the primary data obtained in a kinetic experiment with E. coli cells, focusing on the expression of the motility gene tar in a mutant background. A: Absorbance (●, black) and fluorescence (●, blue) data, corrected for background intensities, obtained with the ΔcpxR strain transformed with the ptar-gfp reporter plasmid and grown in M9 with glucose. B: Activity of the tar promoter, computed from the primary data. The solid black line corresponds to the mean of 6 replicate absorbance measurements and the shaded blue region to the mean of the promoter activities ± twice the standard error of the mean.

The specific niche of IBIS in the field of network inference has been the development and application of genome engineering techniques for constructing the reporter and perturbation systems described above, as well as the use of reporter gene data for the reconstruction of gene regulation functions. We have developed an experimental pipeline that resolves most technical difficulties in the generation of reproducible time-series measurements on the population level. The pipeline comes with data analysis software that converts the primary data into measurements of time-varying promoter activities (Sections 5.4 and 5.3). In addition, for measuring gene expression on the single-cell level by means of microfluidics and time-lapse fluorescence microscopy, we have established collaborations with groups in Grenoble and Paris. The data thus obtained can be exploited for the structural and parametric identification of gene regulatory networks, for which methods with a solid mathematical foundation are developed, in collaboration with colleagues at ETH Zürich and EPF Lausanne (Switzerland). The vertical integration of the network inference process, from the construction of the biological material to the data analysis and inference methods, has the advantage that it allows the experimental design to be precisely tuned to the identification requirements.

3.3. Analysis of integrated metabolic and gene regulatory networks

Participants: Eugenio Cinquemani, Hidde de Jong, Thibault Etienne, Johannes Geiselmann, Stephan Lacour, Yves Markowicz, Aline Métris, Michel Page, Corinne Pinel, Delphine Ropers [Correspondent].

The response of bacteria to changes in their environment involves responses on several different levels, from the redistribution of metabolic fluxes and the adjustment of metabolic pools to changes in gene expression. In order to fully understand the mechanisms driving the adaptive response of bacteria, as mentioned above, we need to analyze the interactions between metabolism and gene expression. While often studied in isolation, gene regulatory networks and metabolic networks are closely intertwined. Genes code for enzymes which control metabolic fluxes, while the accumulation or depletion of metabolites may affect the activity of transcription factors and thus the expression of enzyme-encoding genes.

The fundamental principles underlying the interactions between gene expressions and metabolism are far from being understood today. From a biological point of view, the problem is quite challenging, as metabolism and gene expression are dynamic processes evolving on different time-scales and governed by different types of kinetics. Moreover, gene expression and metabolism are measured by different experimental methods generating heterogeneous, and often noisy and incomplete data sets. From a modeling point of view, difficult methodological problems concerned with the reduction and calibration of complex nonlinear models need to be addressed.

Most of the work carried out within the IBIS project-team specifically addressed the analysis of integrated metabolic and gene regulatory networks in the context of *E. coli* carbon metabolism (Figure 4). While an enormous amount of data has accumulated on this model system, the complexity of the regulatory mechanisms and the difficulty to precisely control experimental conditions during growth transitions leave many essential questions open, such as the physiological role and the relative importance of mechanisms on different levels of regulation (transcription factors, metabolic effectors, global physiological parameters, ...). We are interested in the elaboration of novel biological concepts and accompanying mathematical methods to grasp the nature of the interactions between metabolism and gene expression, and thus better understand the overall functioning of the system. Moreover, we have worked on the development of methods for solving what is probably the hardest problem when quantifying the interactions between metabolism and gene expression: the estimation of parameters from hetereogeneous and noisy high-throughput data. These problems are tackled in collaboration with experimental groups at Inra/INSA Toulouse and CEA Grenoble, which have complementary experimental competences (proteomics, metabolomics) and biological expertise.

3.4. Natural and engineered control of growth and gene expression

Participants: Célia Boyat, Eugenio Cinquemani, Cyril Dutrieux, Johannes Geiselmann [Correspondent], Nils Giordano, Hidde de Jong, Stephan Lacour, Ludowic Lancelot, Delphine Ropers, Alberto Soria-Lopéz.

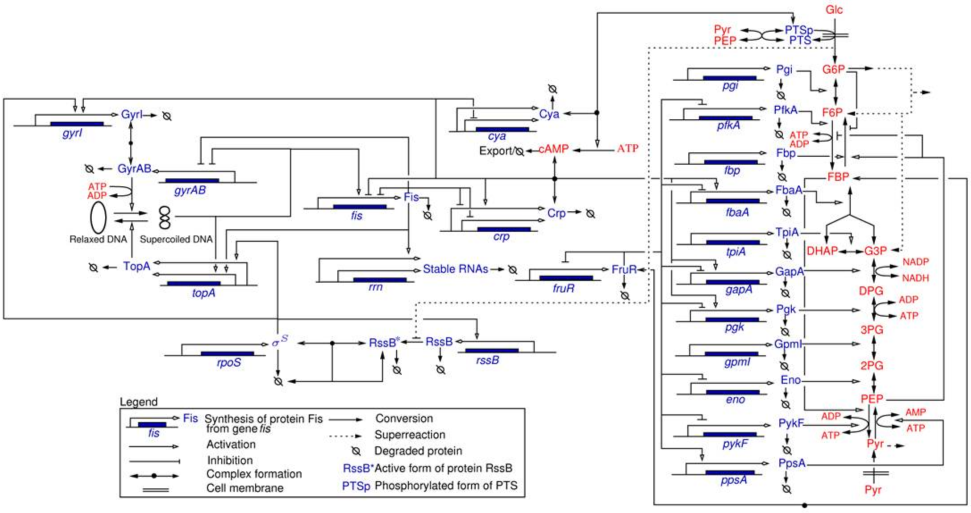


Figure 4. Network of key genes, proteins, and regulatory interactions involved in the carbon assimilation network in E. coli (Baldazzi et al., PLoS Computational Biology, 6(6):e1000812, 2010). The metabolic part includes the glycolysis/gluconeogenesis pathways as well as a simplified description of the PTS system, via the phosphorylated and non-phosphorylated form of its enzymes (represented by PTSp and PTS, respectively). The pentose-phosphate pathway (PPP) is not explicitly described but we take into account that a small pool of G6P escapes the upper part of glycolysis. At the level of the global regulators the network includes the control of the DNA supercoiling level, the accumulation of the sigma factor RpoS and the Crp·cAMP complex, and the regulatory role exerted by the fructose repressor FruR.

The adaptation of bacterial physiology to changes in the environment, involving changes in the growth rate and a reorganization of gene expression, is fundamentally a resource allocation problem. It notably poses the question how microorganisms redistribute their protein synthesis capacity over different cellular functions when confronted with an environmental challenge. Assuming that resource allocation in microorganisms has been optimized through evolution, for example to allow maximal growth in a variety of environments, this question can be fruitfully formulated as an optimal control problem. We have developed such an optimal control perspective, focusing on the dynamical adaptation of growth and gene expression in response to envrionmental changes, in close collaboration with the BIOCORE project-team.

A complementary perspective consists in the use of control-theoretical approaches to modify the functioning of a bacterial cell towards a user-defined objective, by rewiring and selectively perturbing its regulatory networks. The question how regulatory networks in microorganisms can be externally controlled using engineering approaches has a long history in biotechnology and is receiving much attention in the emerging field of synthetic biology. Within a number of on-going projects, IBIS is focusing on two different questions. The first concerns the development of open-loop and closed-loop growth-rate controllers of bacterial cells for both fundamental research and biotechnological applications (Figure 5). Second, we are working on the development of methods for the real-time control of gene expression. These methods are obviously capital for the above-mentioned design of growth-rate controllers, but they have also been applied in the context of a platform for real-time control of gene expression in cell population and single cells, developed by the Inria project-team LIFEWARE, in collaboration with a biophysics group at Université Paris Descartes.

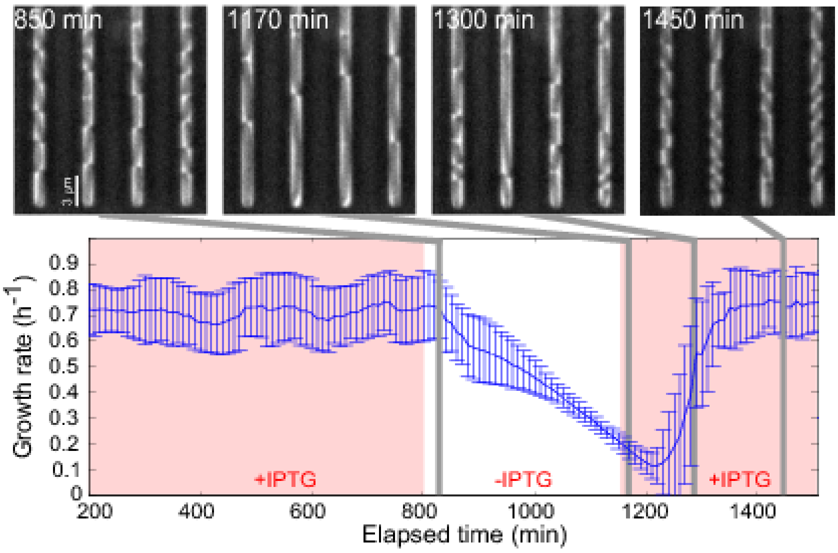


Figure 5. Growth arrest by external control of the gene expression machinery (Izard, Gomez Balderas et al., Molecular Systems Biology, 11:840, 2015). An E. coli strain in which an essential component of the gene expression machinery, the $\beta\beta'$ subunits of RNA polymerase, was put under the control of an externally-supplied inducer (IPTG), was grown in a microfluidics device and phase-contrast images were acquired every 10 min. The cells were grown in minimal medium with glucose, initially in the presence of 1 mM IPTG. 6 h after removing IPTG from the medium, the growth rate slows down and cells are elongated. About 100 min after adding back 1 mM IPTG into the medium, the elongated cells divide and resume normal growth. The growth rates in the plot are the (weighted) mean of the growth rates of 100 individual cells. The error bars correspond to ± one standard deviation. The results of the experiment show that the growth rate of a bacterial can be switched off in a reversible manner by an external inducer, based on the reengineering of the natural control of the expression of RNA polymerase.

LEMON Team

3. Research Program

3.1. State of the Art

3.1.1. Shallow Water Models

Shallow Water (SW) wave dynamics and dissipation represent an important research field. This is because shallow water flows are the most common flows in geophysics. In shallow water regions, dispersive effects (non-hydrostatic pressure effects related to strong curvature in the flow streamlines) can become significant and affect wave transformations. The shoaling of the wave (the "steepening" that happens before the breaking) cannot be described with the usual Saint-Venant equations. To model such various evolutions, one has to use more sophisticated models (Boussinesq, Green-Naghdi...). Nowadays, the classical Saint-Venant equations can be solved numerically in an accurate way, allowing the generation of bores and the shoreline motion to be handled, using recent finite-volume or discontinuous-Galerkin schemes. In contrast, very few advanced works regarding the derivation and modern numerical solution of dispersive equations [23], [27], [56] are available in one dimensions, let alone in the multidimensional case. We can refer to [55], [30] for some linear dispersive equations, treated with finite-element methods, or to [27] for the first use of advanced high-order compact finite-volume methods for the Serre equations. Recent work undertaken during the ANR MathOCEAN [23] lead to some new 1D fully nonlinear and weakly dispersive models (Green-Naghdi like models) that allow to accurately handle the nonlinear waves transformations. High order accuracy numerical methods (based on a second-order splitting strategy) have been developed and implemented, raising a new and promising 1D numerical model. However, there is still a lack of new development regarding the multidimensional case.

In shallow water regions, depending on the complex balance between non-linear effects, dispersive effects and energy dissipation due to wave breaking, wave fronts can evolve into a large range of bore types, from purely breaking to purely undular bore. Boussinesq or Green-Naghdi models can handle these phenomena [21] . However, these models neglect the wave overturning and the associated dissipation, and the dispersive terms are not justified in the vicinity of the singularity. Previous numerical studies concerning bore dynamics using depth-averaged models have been devoted to either purely broken bores using NSW models [24], or undular bores using Boussinesq-type models [34]. Let us also mention [32] for tsunami modeling and [31], [43] for the dam-break problem. A model able to reproduce the various bore shapes, as well as the transition from one type of bore to another, is required. A first step has been made with the one-dimensional code [23], [53]. The SWASH project led by Zijlema at Delft [56] addresses the same issues.

3.1.2. Open boundary conditions and coupling algorithms

For every model set in a bounded domain, there is a need to consider boundary conditions. When the boundaries correspond to a modeling choice rather than to a physical reality, the corresponding boundary conditions should not create spurious oscillations or other unphysical behaviour at the artificial boundary. Such conditions are called **open boundary conditions** (OBC). They have been widely studied by applied mathematicians since the pionneering work of [33] on transparent boundary conditions. Deep studies of these operators have been performed in the case of linear equations, [38], [22], [50]. Unfortunately, in the case of geophysical fluid dynamics, this theory leads to nonlocal conditions (even in linear cases) that are not usable in numerical models. Most of current models (including high quality operational ones) modestly use a *no flux* condition (namely an homogeneous Neumann boundary condition) when a free boundary condition is required. But in many cases, Neumann homogeneous conditions are a very poor approximation of the exact transparent conditions. Hence the need to build higher order approximations of these conditions that remain numerically tractable.

Numerous physical processes are involved in coastal modeling, each of them depending on others (surface winds for coastal oceanography, sea currents for sandbars dynamics, etc.). Connecting two (or more) model solutions at their interface is a difficult task, that is often addressed in a simplified way from the mathematical viewpoint: this can be viewed as the one and only iteration of an iterative process. This results with a low quality coupled system, which could be improved either with additional iterations, and/or thanks to the improvement of interface boundary conditions and the use of OBC (see above). Promising results have been obtained in the framework of **ocean-atmosphere coupling** (in a simplified modeling context) in [44], where the use of advanced coupling techniques (based on domain decomposition algorithm) are introduced.

3.1.3. A need for upscaled shallow water models.

The mathematical modeling of **fluid-biology** coupled systems in lagoon ecosystems requires one or several water models. It is of course not necessary (and not numerically feasible) to use accurate non-hydrostatic turbulent models to force the biological processes over very long periods of time. There is a compromise to be reached between accurate (but untractable) fluid models such as the Navier-Stokes equations and simple (but imprecise) models such as [35].
In urbanized coastal zones, upscaling is also a key issue. This stems not only from the multi-scale aspects dealt with in the previous subsection, but also from modeling efficiency considerations.

The typical size of the relevant hydraulic feature in an urban area is between 0.1 m and 1.0 m, while the size of an urban area usually ranges from 10^3 m to 10^4 m. Refined flow computations (e.g. in simulating the impact of a tsunami) over entire coastal conurbations using a 2D horizontal model thus require 10^6 to 10^9 elements. From an engineering perspective, this makes both the CPU and man-supervised mesh design efforts unaffordable in the present state of technology.

Upscaling provides an answer to this problem by allowing macroscopic equations to be derived from the small-scale governing equations. The powerful, multiple scale expansion-based homogeneization technique [20], [19], [49] has been applied successfully to flow and transport upscaling in porous media, but its use is subordinated to the stringent assumptions of (i) the existence of a Representative Elementary Volume (REV), (ii) the scale separation principle, and (iii) the process is not purely hyperbolic at the microscopic scale, otherwise precluding the study of transient solutions [20]. Unfortunately, the REV has been shown recently not to exist in urban areas [37]. Besides, the scale separation principle is violated in the case of sharp transients (such as tsunami waves) impacting urban areas because the typical wavelength is of the same order of magnitude as the microscopic detail (the street/block size). Moreover, 2D shallow water equations are essentially hyperbolic, thus violating the third assumption.

These hurdles are overcome by averaging approaches. Single porosity-based, macroscopic shallow water models have been proposed [29], [36], [39] and applied successfully to urban flood modeling scale experiments [36], [45], [52]. They allow the CPU time to be divided by 10 to 100 compared to classical 2D shallow water models. Recent extensions of these models have been proposed in the form of integral porosity [51] and multiple porosity [37] shallow water models.

3.2. Scientific Objectives

Our main challenge is: build and couple elementary models in coastal areas to improve their capacity to simulate complex dynamics. This challenge consists of three principal scientific objectives. First of all, each of the elementary models has to be consistently developed (regardless of boundary conditions and interactions with other processes). Then open boundary conditions (for the simulation of physical processes in bounded domains) and links between the models (interface conditions) have to be identified and formalized. Finally, models and boundary conditions (*i.e.* coupled systems) should be proposed, analyzed and implemented in a common platform.

3.2.1. Single process models and boundary conditions

The time-evolution of a water flow in a three-dimensional computational domain is classically modeled by Navier-Stokes equations for incompressible fluids. Depending on the physical description of the considered domain, these equations can be simplified or enriched. Consequently, there are **numerous water dynamics models** that are derived from the original Navier-Stokes equations, such as primitive equations, shallow water equations (see [28]), Boussinesq-type dispersive models [21]), etc. The aforementioned models have **very different mathematical natures**: hyperbolic *vs* parabolic, hydrostatic *vs* non-hydrostatic, inviscid *vs* viscous, etc. They all carry nonlinearities that make their mathematical study (existence, uniqueness and regularity of weak and/or strong solutions) highly challenging (not to speak about the $1M Clay competition for the 3D Navier Stokes equations, which may remain open for some time).

The objective is to focus on the mathematical and numerical modeling of models adapted to **nearshore dynamics**, accounting for complicated wave processes. There exists a large range of models, from the shallow water equations (eventually weakly dispersive) to some fully dispersive deeper models. All these models can be obtained from a suitable asymptotic analysis of the water wave equations (Zakharov formulation) and if the theoretical study of these equations has been recently investigated [42], there is still some serious numerical challenges. So we plan to focus on the derivation and implementation of robust and high order discretization methods for suitable two dimensional models, including enhanced fully nonlinear dispersive models and fully dispersive models, like the Matsuno-generalized approach proposed in [41]. Another objective is to study the shallow water dispersive models without any irrotational flow assumption. Such a study would be of great interest for the study of nearshore circulation (wave induced rip currents).

For obvious physical and/or computational reasons, our models are set in bounded domains. Two types of boundaries are considered: physical and mathematical. Physical boundaries are materialized by an existing interface (atmosphere/ocean, ocean/sand, shoreline, etc.) whereas mathematical boundaries appear with the truncation of the domain of interest. In the latter case, **open boundary conditions** are mandatory in order not to create spurious reflexions at the boundaries. Such boundary conditions being nonlocal and impossible to use in practice, we shall look for approximations. We shall obtain them thanks to the asymptotic analysis of the (pseudo-differential) boundary operators with respect to small parameters (viscosity, domain aspect ratio, Rossby number, etc.). Naturally, we **will seek the boundary conditions leading to the best compromise** between mathematical well-posedness and physical consistency. This will make extensive use of the mathematical theory of **absorbing operators** and their approximations [33].

3.2.2. Coupled systems

The Green-Naghdi equations provide a correct description of the waves up to the breaking point while the Saint-Venant equations are more suitable for the description of the surf zone (i.e. after the breaking). Therefore, the challenge here is first to **design a coupling strategy** between these two systems of equations, first in a simplified one-dimensional case, then to the two-dimensional case both on cartesian and unstructured grids. High order accuracy should be achieved through the use of flexible Discontinuous-Galerkin methods.
Additionally, we will couple our weakly dispersive shallow water models to other fully dispersive deeper water models. We plan to mathematically analyze the coupling between these models. In a first step, we have to understand well the mixed problem (initial and boundary conditions) for these systems. In a second step, these new mathematical development have to be embedded within a numerically efficient strong coupling approach. The deep water model should be fully dispersive (solved using spectral methods, for instance) and the shallow-water model will be, in a first approach, the Saint-Venant equations. Then, when the 2D extension of the currently developped Green-Naghdi numerical code will be available, the improved coupling with a weakly dispersive shallow water model should be considered.

In the context of Schwarz relaxation methods, usual techniques can be seen as the first iteration (not converged) of an iterative algorithm. Thanks to the work performed on efficient boundary conditions, we shall **improve the quality of current coupling algorithms**, allowing for qualitatively satisfying solutions **with a reduced computational cost** (small number of iterations).

We are also willing to explore the role of geophysical processes on some biological ones. For example, the design of optimal shellfish farms relies on confinement maps and plankton dynamics, which strongly depend on long-time averaged currents. Equations that model the time evolution of species in a coastal ecosystem are relatively simple from a modeling viewpoint: they mainly consist of ODEs, and possibly advection-diffusion equations. The issue we want to tackle is the choice of the fluid model that should be coupled to them, accounting for the important time scales discrepancy between biological (evolution) processes and coastal fluid dynamics. Discrimination criteria between refined models (such as turbulent Navier-Stokes) and cheap ones (see [35]) will be proposed.

Coastal processes evolve at very different time scales: atmosphere (seconds/minutes), ocean (hours), sediment (months/years) and species evolution (years/decades). Their coupling can be seen as a *slow-fast* dynamical system, and a naïve way to couple them would be to pick the smallest time-step and run the two models together: but the computational cost would then be way too large. Consequently **homogenization techniques or other upscaling methods** should be used in order to account for these various time scales at an affordable computational cost. The research objectives are the following:

- So far, the proposed upscaled models have been validated against theoretical results obtained from refined 2D shallow water models and/or very limited data sets from scale model experiments. The various approaches proposed in the literature [25], [26], [29], [36], [37], [39], [45], [51], [52] have not been compared over the same data sets. Part of the research effort will focus on the extensive validation of the models on the basis of scale model experiments. Active cooperation will be sought with a number of national and international Academic partners involved in urban hydraulics (UCL Louvain-la-Neuve, IMFS Strasbourg, Irvine University California) with operational experimental facilities.
- Upscaling of source terms. Two types of source terms play a key role in shallow water models: geometry-induced source terms (arising from the irregular bathymetry) and friction/turbulence-induced energy loss terms. In all the upscaled shallow water models presented so far, only the large scale effects of topographical variations have been upscaled. In the case of wetting/drying phenomena and small depths (e.g. the *Camargue* tidal flats), however, it is forseen that subgrid-scale topographic variations may play a predominant role. Research on the integration of subgrid-scale topography into macrosocopic shallow water models is thus needed. Upscaling of friction/turbulence-induced head loss terms is also a subject for research, with a number of competing approaches available from the literature [36], [37], [51], [54].
- Upscaling of transport processes. The upscaling of surface pollutant transport processes in the urban environment has not been addressed so far in the literature. Free surface flows in urban areas are characterized by strongly variable (in both time and space) flow fields. Dead/swirling zones have been shown to play a predominant role in the upscaling of the flow equations [37], [51]. Their role is expected to be even stronger in the upscaling of contaminant transport. While numerical experiments indicate that the microscopic hydrodynamic time scales are small compared to the macroscopic time scales, theoretical considerations indicate that this may not be the case with scalar transport. Trapping phenomena at the microscopic scale are well-known to be upscaled in the form of fractional dynamics models in the long time limit [40], [47]. The difficulty in the present research is that upscaling is not sought only for the long time limit but also for all time scales. Fractional dynamics will thus probably not suffice to a proper upscaling of the transport equations at all time scales.

3.2.3. Numerical platform

As a long term objective, the team shall create a common architecture for existing codes, and also the future codes developed by the project members, to offer a simplified management of various evolutions and a single and well documented tool for our partners. It will aim to be self-contained including pre and post-processing tools (efficient meshing approaches, GMT and VTK libraries), but must of course also be opened to user's suggestions, and account for existing tools inside and outside Inria. This numerical platform will be dedicated to the simulation of all the phenomena of interest, including flow propagation, sediment evolution, model coupling on large scales, from deep water to the shoreline, including swell propagation, shoaling, breaking and run-up. This numerical platform clearly aims at becoming a reference software in the community. It should be used to **develop a specific test case** around Montpellier which embeds many processes and their mutual interactions: from the *Camargue* (where the Rhône river flows into the Mediterranean sea) to the *Étang de Thau* (a wide lagoon where shellfishes are plentiful), **all the processes studied in the project occur in a 100km wide region**, including of course the various hydrodynamics regimes (from the deep sea to the shoaling, surf and swash zones) and crucial morphodynamic issues (*e.g.* in the town of Sete).

LIFEWARE Project-Team

3. Research Program

3.1. Computational Systems Biology

Bridging the gap between the complexity of biological systems and our capacity to model and **quantitatively predict system behaviors** is a central challenge in systems biology. We believe that a deeper understanding of the concept and theory of biochemical computation is necessary to tackle that challenge. Progress in the theory is necessary for scaling, and enabling the application of static analysis, module identification and decomposition, model reductions, parameter search, and model inference methods to large biochemical reaction systems. A measure of success on this route will be the production of better computational modeling tools for elucidating the complex dynamics of natural biological processes, designing synthetic biological circuits and biosensors, developing novel therapy strategies, and optimizing patient-tailored therapeutics.

Progress on the **coupling of models to data** is also necessary. Our approach based on quantitative temporal logics provides a powerful framework for formalizing experimental observations and using them as formal specification in model building. Key to success is a tight integration between *in vivo* and *in silico* work, and on the mixing of dry and wet experiments, enabled by novel biotechnologies. In particular, the use of microfluidic devices makes it possible to measure behaviors at both single-cell and cell population levels *in vivo*, provided innovative modeling, analysis and control methods are deployed *in silico*.

In synthetic biology, while the construction of simple intracellular circuits has shown feasible, the design of larger, **multicellular systems** is a major open issue. In engineered tissues for example, the behavior results from the subtle interplay between intracellular processes (signal transduction, gene expression) and intercellular processes (contact inhibition, gradient of diffusible molecule), and the question is how should cells be genetically modified such that the desired behavior robustly emerges from cell interactions.

3.2. Modeling of Phenotypic Heterogeneity in Cellular Processes

Since nearly two decades, a significant interest has grown for getting a quantitative understanding of the functioning of biological systems at the cellular level. Given their complexity, proposing a model accounting for the observed cell responses, or better, predicting novel behaviors, is now regarded as an essential step to validate a proposed mechanism in systems biology. Moreover, the constant improvement of stimulation and observation tools creates a strong push for the development of methods that provide predictions that are increasingly precise (single cell precision) and robust (complex stimulation profiles).

It is now fully apparent that cells do not respond identically to a same stimulation, even when they are all genetically-identical. This phenotypic heterogeneity plays a significant role in a number of problems ranging from cell resistance to anticancer drug treatments to stress adaptation and bet hedging.

Dedicated modeling frameworks, notably **stochastic** modeling frameworks, such as chemical master equations, and **statistic** modeling frameworks, such as ensemble models, are then needed to capture biological variability.

Appropriate mathematical and computational should then be employed for the analysis of these models and their calibration to experimental data. One can notably mention **global optimization** tools to search for appropriate parameters within large spaces, **moment closure** approaches to efficiently approximate stochastic models [0], and (stochastic approximations of) the **expectation maximization** algorithm for the identification of mixed-effects models [0].

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3.3. Logical Paradigm for Systems Biology

Our group was among the first ones in 2002 to apply **model-checking** methods to systems biology in order to reason on large molecular interaction networks, such as Kohn's map of the mammalian cell cycle (800 reactions over 500 molecules) [0]. The logical paradigm for systems biology that we have subsequently developed for quantitative models can be summarized by the following identifications :

$$\text{biological model = transition system } K$$

$$\text{dynamical behavior specification = temporal logic formula } \phi$$

$$\text{model validation = model-checking } \quad K,\ s \models ?\ \phi$$

$$\text{model reduction = sub-model-checking } \quad K'? \subset K,\ K',\ s \models \phi$$

$$\text{model prediction = formula enumeration } \quad K,\ s \models \phi ?$$

$$\text{static experiment design = symbolic model-checking } \quad K,\ s? \models \phi$$

$$\text{model inference = constraint solving } \quad K?,\ s \models \phi$$

$$\text{dynamic experiment design = constraint solving } \quad K?,\ s? \models \phi$$

In particular, the definition of a continuous satisfaction degree for **first-order temporal logic** formulae with constraints over the reals, was the key to generalize this approach to quantitative models, opening up the field of model-checking to model optimization [0] This line of research continues with the development of temporal logic patterns with efficient constraint solvers and their generalization to handle stochastic effects.

3.4. External Control of Cell Processes

External control has been employed since many years to regulate culture growth and other physiological properties. Recently, taking inspiration from developments in synthetic biology, closed loop control has been applied to the regulation of intracellular processes. Such approaches offer unprecedented opportunities to investigate how a cell process dynamical information by maintaining it around specific operating points or driving it out of its standard operating conditions. They can also be used to complement and help the development of synthetic biology through the creation of hybrid systems resulting from the interconnection of in vivo and in silico computing devices.

In collaboration with Pascal Hersen (CNRS MSC lab), we developed a platform for gene expression control that enables to control protein concentrations in yeast cells. This platform integrates microfluidic devices enabling long-term observation and rapid change of the cells environment, microscopy for single cell measurements, and software for real-time signal quantification and model based control. We demonstrated recently that this platform enables controlling the level of a fluorescent protein in cells with unprecedented accuracy and for many cell generations [0].

More recently, motivated by an analogy with a benchmark control problem, the stabilization of an inverted pendulum, we investigated the possibility to balance a genetic toggle switch in the vicinity of its unstable equilibrium configuration. We searched for solutions to balance an individual cell and even an entire population of heterogeneous cells, each harboring a toggle switch.

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3.5. Chemical Reaction Network Theory

Feinberg's chemical reaction network theory and Thomas's influence network analyses provide sufficient and/or necessary structural conditions for the existence of multiple steady states and oscillations in regulatory networks, which can be predicted by static analyzers without making any simulation. In this domain, most of our work consists in analyzing the interplay between the **structure** (Petri net properties, influence graph, subgraph epimorphisms) and the **dynamics** (Boolean, CTMC, ODE, time scale separations) of biochemical reaction systems. In particular, our study of influence graphs of reaction systems, our generalization of Thomas' conditions of multi-stationarity and Soulé's proof to reaction systems [0], the inference of reaction systems from ODEs [0], the computation of structural invariants by constraint programming techniques, and the analysis of model reductions by subgraph epimorphisms now provide solid ground for developing static analyzers, using them on a large scale in systems biology, and elucidating modules.

3.6. Mixed Analog-Digital Computation with Biochemical Reactions

The continuous nature of many protein interactions leads us to consider models of analog computation, and in particular, the recent results in the theory of analog computability and complexity obtained by Amaury Pouly [0] and Olivier Bournez, establish fundamental links with digital computation. In [18], we derive from these results a Turing completeness result for elementary reaction systems (without polymerization) under the differential semantics. The proof of this result shows how mathematical functions described by Ordinary Differential Equations, namely by Polynomial Initial Value Problems (PIVP), can be compiled into elementary biochemical reactions, furthermore with a notion of analog computation complexity defined as the length of the trajectory to reach a given precision on the result. This opens a whole research avenue to analyze natural circuits in Systems Biology, transform behavioural specifications into biochemical reactions for Synthetic Biology, and compare artificial circuits with natural circuits acquired through evolution, from the novel point of view of analog computation complexity.

3.7. Constraint Solving and Optimization

Constraint solving and optimization methods are important in our research [17]. On the one hand, static analysis of biochemical reaction networks involves solving hard combinatorial optimization problems, for which **constraint programming** techniques have shown particularly successful, often beating dedicated algorithms and allowing to solve large instances from model repositories. On the other hand, parameter search and model calibration problems involve similarly solving hard continuous optimization problems, for which **evolutionary algorithms** such as the covariance matrix evolution strategy (CMA-ES) [0] has shown to provide best results in our context, for up to 100 parameters, for building challenging quantitative models, gaining model-based insights, revisiting admitted assumptions, and contributing to biological knowledge [0].

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M3DISIM Project-Team

3. Research Program

3.1. Multi-scale modeling and coupling mechanisms for biomechanical systems, with mathematical and numerical analysis

Over the past decade, we have laid out the foundations of a multi-scale 3D model of the cardiac mechanical contraction responding to electrical activation. Several collaborations have been crucial in this enterprise, see below references. By integrating this formulation with adapted numerical methods, we are now able to represent the whole organ behavior in interaction with the blood during complete heart beats. This subject was our first achievement to combine a deep understanding of the underlying physics and physiology and our constant concern of proposing well-posed mathematical formulations and adequate numerical discretizations. In fact, we have shown that our model satisfies the essential thermo-mechanical laws, and in particular the energy balance, and proposed compatible numerical schemes that – in consequence – can be rigorously analyzed, see [5]. In the same spirit, we have recently formulated a poromechanical model adapted to the blood perfusion in the heart, hence precisely taking into account the large deformation of the mechanical medium, the fluid inertia and moving domain, and so that the energy balance between fluid and solid is fulfilled from the model construction to its discretization, see [6].

3.2. Inverse problems with actual data – Fundamental formulation, mathematical analysis and applications

A major challenge in the context of biomechanical modeling – and more generally in modeling for life sciences – lies in using the large amount of data available on the system to circumvent the lack of absolute modeling ground truth, since every system considered is in fact patient-specific, with possibly non-standard conditions associated with a disease. We have already developed original strategies for solving this particular type of inverse problems by adopting the observer stand-point. The idea we proposed consists in incorporating to the classical discretization of the mechanical system an estimator filter that can use the data to improve the quality of the global approximation, and concurrently identify some uncertain parameters possibly related to a diseased state of the patient, see [7], [8], [9]. Therefore, our strategy leads to a coupled model-data system solved similarly to a usual PDE-based model, with a computational cost directly comparable to classical Galerkin approximations. We have already worked on the formulation, the mathematical and numerical analysis of the resulting system – see [3] – and the demonstration of the capabilities of this approach in the context of identification of constitutive parameters for a heart model with real data, including medical imaging, see [1].

MAGIQUE-3D Project-Team

3. Research Program

3.1. Introduction

Probing the invisible is a quest that is shared by a wide variety of scientists such as archaeologists, geologists, astrophysicists, physicists, etc... Magique-3D is involved in Geophysical imaging which aims at understanding the internal structure of the Earth from the propagation of waves. Both qualitative and quantitative information are required and two geophysical techniques can be used: **seismic reflection** and **seismic inversion**. Seismic reflection provides a qualitative description of the subsurface from reflected seismic waves by indicating the position of the reflectors while seismic inversion transforms seismic reflection data into a quantitative description of the subsurface. Both techniques are inverse problems based upon the numerical solution of wave equations. Oil and Gas explorations have been pioneering application domains for seismic reflection and inversion and even if numerical seismic imaging is computationally intensive, oil companies promote the use of numerical simulations to provide synthetic maps of the subsurface. This is due to the tremendous progresses of scientific computing which have pushed the limits of existing numerical methods and it is now conceivable to tackle realistic 3D problems. However, mathematical wave modeling has to be well-adapted to the region of interest and the numerical schemes which are employed to solve wave equations have to be both accurate and scalable enough to take full advantage of parallel computing. Today, geophysical imaging tackles more and more realistic problems and we can contribute to this task by improving the modeling and by deriving advanced numerical methods for solving wave problems.

Magique-3D proposes to organize its research around three main axes:

1. Mathematical modeling of multi-physics involving wave equations;
2. Supercomputing for Helmholtz problems;
3. Construction of high-order hybrid schemes.

These three research fields will be developed with the main objective of solving inverse problems dedicated to geophysical imaging.

3.2. Mathematical modeling of multi-physics involving wave equations

Wave propagation modeling is of great interest for many applications like oil and gas exploration, non destructive testing, medical imaging, etc. It involves equations which can be solved in time or frequency domain and their numerical approximation is not easy to handle, in particular when dealing with real-world problems. In both cases, the propagation domain is either infinite or its dimensions are much greater than the characteristic wavelength of the phenomenon of interest. But since wave problems are hyperbolic, the physical phenomenon can be accurately described by computing solutions in a bounded domain including the sources which have generated the waves. Until now, we have mainly worked on imaging techniques based on acoustic or elastic waves and we have developed advanced finite element software packages which are used by Total for oil exploration. Nevertheless, research on modeling must go on because there are simulations which can still not be performed because their computational cost is much too high. This is particularly true for complex tectonics involving coupled wave equations. We then propose to address the issue of coupling wave equations problems by working on the mathematical construction of reduced systems. By this way, we hope to improve simulations of elasto-acoustic and electro-seismic phenomena and then, to perform numerical imaging of strongly heterogeneous media. Even in the simplest situation where the wavelengths are similar (elasto-acoustic coupling), the dimension of the discrete coupled problem is huge and it is a genuine issue in the prospect of solving 3D inverse problems.

The accurate numerical simulation of full wave problems in heterogeneous media is computationally intensive since it needs numerical schemes based on grids. The size of the cells depends on the propagation velocity of waves. When coupling wave problems, conversion phenomena may occur and waves with very different propagation velocity coexist. The size of the cells is then defined from the smallest velocity and in most of the real-world cases, the computational cost is crippling. Regarding existing computing capabilities, we propose to derive intermediate models which require less computational burden and provide accurate solutions for a wide-ranging class of problems including Elasto-acoustics and Electro-seismology.

When it comes to mathematical analysis, we have identified two tasks which could help us simulate realistic 3D multi-physics wave problems and which are in the scope of our savoir-faire. They are construction of approximate and multiscale models which are different tasks. The construction of approximate problems aims at deriving systems of equations which discrete formulation involves middle-sized matrices and in general, they are based on high frequency hypothesis. Multiscale models are based on a rigorous analysis involving a small parameter which does not depend on the propagation velocity necessarily.

Recently, we have conducted research on the construction of approximate models for offshore imaging. Elastic and acoustic wave equations are coupled and we investigate the idea of eliminating the computations inside water by introducing equivalent interface conditions on the sea bottom. We apply an On-Surface-Radiation-Condition (OSRC) which is obtained from the approximation of the acoustic Dirichlet-to-Neumann (DtN) operator [74], [53]. To the best of our knowledge, OSRC method has never been used for solving reduced coupling wave problems and preliminary promising results are available at [56]. We would like to investigate this technique further because we could form a battery of problems which can be solved quickly. This would provide a set of solutions which we could use as initial guess for solving inverse problems. But we are concerned with the performance of the OSRC method when wave conversions with different wavelengths occur. Anyway, the approximation of the DtN operator is not obvious when the medium is strongly heterogeneous and multiscale analysis might be more adapted. For instance, according to existing results in Acoustics and Electromagnetism for the modeling of wire antennas [65], multiscale analysis should turn out to be very efficient when the propagation medium includes well logs, fractures and faults which are very thin structures when compared to the wavelength of seismic waves. Moreover, multiscale analysis should perform well when the medium is strongly oscillating like porous media. It could thus provide an alternative to homogenization techniques which can be applied only when the medium is periodic. We thus propose to develop reduced multi-scale models by performing rigorous mathematical procedure based on regular and singular multiscale analysis. Our approach distinguishes itself from others because it focuses on the numerical representation of small structures by time-dependent problems. This could give rise to the development of new finite element methods which would combine DG approximations with XFEM (Extended Finite Element Method) which has been created for the finite element treatment of thin structures like cracks.

But Earth imaging must be more than using elasto-acoustic wave propagation. Electromagnetic waves can also be used and in collaboration with Prof. D. Pardo (Iker Basque Foundation and University of Bilbao), we conduct researches on passive imaging to probe boreholes. Passive imaging is a recent technique of imaging which uses natural electromagnetic fields as sources. These fields are generated by hydromagnetic waves propagating in the magnetosphere which transform into electromagnetic waves when they reach the ionosphere. This is a mid-frequency imaging technique which applies also to mineral and geothermal exploration, to predict seismic hazard or for groundwater monitoring. We aim at developing software package for resistivity inversion, knowing that current numerical methods are not able to manage 3D inversion. We have obtained results based on a Petrov-Galerkin approximation [50], but they are limited to 2D cases. We have thus proposed to reduce the 3D problem by using 1D semi-analytic approximation of Maxwell equations [78]. This work has just started in the framework of a PhD thesis and we hope that it will give us the possibility of imaging 3D problems.

Magique-3D would like to expand its know-how by considering electro-seismic problems which are in the scope of coupling electromagnetic waves with seismic waves. Electro-seismic waves are involved in porous media imaging which is a tricky task because it is based on the coupling of waves with very different wavelengths described by Biot equations and Maxwell equations. Biot equations govern waves in saturated porous media and they represent a complex physical phenomenon involving a slow wave which is very difficult to simulate numerically. In [72], interesting results have been obtained for the simulation of piezoelectric sensors. They are based on a quasi-static approximation of the Maxwell model coupled with Elastodynamics. Now, we are concerned with the capability of using this model for Geophysical Imaging and we believe that the derivation and/or the analysis of suitable modelings is necessary. Collaborations with Geophysicists are thus mandatory in the prospect of using both experimental and numerical approaches. We would like to collaborate with Prof. C. Bordes and Prof. D. Brito (Laboratory of Complex Fluids and their Reservoirs, CNRS and University of Pau) who have efficient experimental devices for the propagation of electromagnetic waves inside saturated porous media [55]. This collaboration should be easy to organize since Magique-3D has a long-term experience in collaborating with geophysicists. We then believe that we will not need a lot of time to get joint results since we can use our advanced software packages Hou10ni and Montjoie and our colleagues have already obtained data. Electro-seismology is a very challenging research domain for us and we would like to enforce our collaborations with IsTerre (Institute of Earth Science, University of Grenoble) and for that topic with Prof. S. Garambois who is an expert in Electro-seismology [80], [81], [69], [70]. A joint research program could gather Geophysicists from the University of Pau and from IsTerre and Magique-3D. In particular, it would be interesting to compare simulations performed with Hou10ni, Montjoie, with the code developed by Prof. S. Garambois and to use experimental simulations for validation.

3.3. Supercomputing for Helmholtz problems

Probing invisible with harmonic equations is a need for many scientists and it is also a topic offering a wealth of interesting problems for mathematicians. It is well-known that Helmholtz equations discretization is very sensitive to the frequency scale which can be wide-ranging for some applications. For example, depth imaging is searching for deeper layers which may contain hydrocarbons and frequencies must be of a few tens of Hertz with a very low resolution. If it is to detect hidden objects, the depth of the explored region does not exceed a few tens of meters and frequencies close to the kiloHertz are used. High performing numerical methods should thus be stable for a widest as possible frequency range. In particular, these methods should minimize phenomena of numerical pollution that generate errors which increase faster with frequency than with the inverse of space discretization step. As a consequence, there is a need of mesh refinement, in particular at high frequency.

During the period 2010-2014, the team has worked extensively on high order discontinuous Galerkin (DG) methods. Like standard Finite Element Methods, they are elaborated with polynomial basis functions and they are very popular because they are defined locally for each element. It is thus easy to use basis polynomial functions with different degrees and this shows the perfect flexibility of the approximation in case of heterogeneous media including homogeneous parts. Indeed, low degree basis functions can be used in heterogeneous regions where a fine grid is necessary while high degree polynomials can be used for coarse elements covering homogeneous parts. In particular, Magique-3D has developed Hou10ni that solves harmonic wave equations with DG methods and curved elements. We found that both the effects of pollution and dispersion, which are very significant when a conventional finite element method is used, are limited [57]. However, bad conditioning is persisting and reliability of the method is not guaranteed when the coefficients vary considerably. In addition, the number of unknowns of the linear system is too big to hope to solve a realistic 3D problem. So it is important to develop approximation methods that require fewer degrees of freedom. Magique-3D wishes to invest heavily in the development of new approximation methods for harmonic wave equations. It is a difficult subject for which we want to develop different tasks, in collaboration with academic researchers with whom we are already working or have established contacts. Research directions that we would like to follow are the following.

First, we will continue our long-term collaboration with Prof. Rabia Djellouli. We want to continue to work on hybrid finite element methods that rely on basis functions composed of plane waves and polynomials. These methods have demonstrated good resistance to the phenomenon of numerical pollution [51], [52], but their capability of solving industrial problems has not been illustrated. This is certainly due to the absence of guideline for choosing the plane waves. We are thus currently working on the implementation of a methodology that makes the choice of plane waves automatic for a given simulation (fixed propagation domain, data source, etc.). This is up-front investigation and there is certainly a lot of remaining work before being applied to geophysical imaging. But it gives the team the opportunity to test new ideas while remaining in contact with potential users of the methods.

Then we want to work with Prof. A. Bendali on developing methods of local integral equations which allow calculation of numerical fluxes on the edges of elements. One could then use these fluxes in a DG method for reconstructing the solution throughout the volume of calculation. This research is motivated by recent results which illustrate the difficulties of the existing methods which are not always able to approximate the propagating modes (plane waves) and the evanescent modes (polynomials) that may coexist, especially when one considers realistic applications. Integral equations are direct tools for computing fluxes and they are known for providing very good accuracy. They thus should help to improve the quality of approximation of DG methods which are fully flux-dependent. In addition, local integral equations would limit calculations at the interfaces, which would have the effect of limiting the number of unknowns generally high, especially for DG methods. Again, it is a matter of long-term research which success requires a significant amount of mathematical analysis, and also the development of non-trivial code.

To limit the effects of pollution and dispersion is not the only challenge that the team wants to tackle. Our experience alongside Total has made us aware of the difficulties in constructing meshes that are essential to achieve our simulations. There are several teams at Inria working on mesh generation and we are in contact with them, especially with Gamma3 (Paris-Rocquencourt Research Center). These teams develop meshes increasingly sophisticated to take account of the constraints imposed by realistic industrial benchmarks. But in our opinion, issues which are caused by the construction of meshes are not the only downside. Indeed, we have in mind to solve inverse problems and in this case it is necessary to mesh the domain at each iteration of Newton-type solver. It is therefore interesting to work on methods that either do not use mesh or rely on meshes which are very easy to construct. Regarding meshless methods, we have begun a collaboration with Prof. Djellouli which allowed us to propose a new approach called Mesh-based Frontier Free Formulation (MF3). The principle of this method is the use of fundamental solutions of Helmholtz equations as basic functions. One can then reduce the volumic variational formulation to a surfacic variational formulation which is close to an integral equation, but which does not require the calculation of singularities. The results are very promising and we hope to continue our study in the context of the application to geophysical imaging. An important step to validate this method will be particularly its extension to 3D because the results we have achieved so far are for 2D problems.

Keeping in mind the idea of limiting the difficulties of mesh, we want to study the method of virtual elements. This method attracts us because it relies on meshes that can be made of arbitrarily-shaped polygon and meshes should thus be fairly straightforward. Existing works on the subject have been mainly developed by the University of Pavia, in collaboration with Los Alamos National Laboratory [54], [61], [60], [58], [62]. None of them mentions the feasibility of the method for industrial applications and to our knowledge, there are no results on the method of virtual elements applied to the wave equations. First, we aim at applying the method described in [59] to the scalar Helmholtz equation and explore opportunities to use discontinuous elements within this framework. Then hp-adaptivity could be kept, which is particularly interesting for wave propagation in heterogeneous media.

DG methods are known to require a lot of unknowns that can exceed the limits accepted by the most advanced computers. This is particularly true for harmonic wave equations that require a large number of discretization points, even in the case of a conventional finite element method. We therefore wish to pursue a research activity that we have just started in collaboration with the project-team Nachos (Sophia-Antipolis Méditerranée Research Center). In order to reduce the number of degrees of freedom, we are interested in "hybrid mixed" Discontinuous Galerkin methods that provides a two-step procedure for solving the Helmholtz equations [73], [77], [76]. First, Lagrange multipliers are introduced to represent the flux of the numerical solution through the interface (edge or face) between two elements. The Lagrange multipliers are solution to a linear system which is constructed locally element by element. The number of degrees of freedom is then strongly reduced since for a standard DG method, there is a need of considering unknowns including volumetric values inside the element. And obviously, the gain is even more important when the order of the element is high. Next, the solution is reconstructed from the values of the multipliers and the cost of this step is negligible since it only requires inverting small-sized matrices. We have obtained promising results in the framework of the PhD

thesis of Marie Bonnasse-Gahot and we want to apply it to the simulation of complex phenomena such as the 3D viscoelastic wave propagation.
Obviously, the success of all these works depends on our ability to consider realistic applications such as wave propagation in the Earth. And in these cases, it is quite possible that even if we manage to develop accurate less expensive numerical methods, the solution of inverse problems will still be computationally intensive. It is thus absolutely necessary that we conduct our research by taking advantage of the latest advances in high-performance computing. We have already initiated discussions with the project team HIEPACS (Bordeaux Sud-Ouest research Center) to test the performance of the latest features of Mumps http://mumps.enseeiht.fr/, such as Low Rank Approximation or adaptation to hybrid CPU / GPU architectures and to Intel Xeon Phi, on realistic test cases. We are also in contact with the team Algorithm at Cerfacs (Toulouse) for the development of local integral equations solvers. These collaborations are essential for us and we believe that they will be decisive for the simulation of three-dimensional elasto-dynamic problems. However, our scientific contribution will be limited in this area because we are not experts in HPC.

3.4. Hybrid time discretizations of high-order

Most of the meshes we consider are composed of cells greatly varying in size. This can be due to the physical characteristics (propagation speed, topography, ...) which may require to refine the mesh locally, very unstructured meshes can also be the result of dysfunction of the mesher. For practical reasons which are essentially guided by the aim of reducing the number of matrix inversions, explicit schemes are generally privileged. However, they work under a stability condition, the so-called Courant Friedrichs Lewy (CFL) condition which forces the time step being proportional to the size of the smallest cell. Then, it is necessary to perform a huge number of iterations in time and in most of the cases because of a very few number of small cells. This implies to apply a very small time step on grids mainly composed of coarse cells and thus, there is a risk of creating numerical dispersion that should not exist. However, this drawback can be avoided by using low degree polynomial basis in space in the small meshes and high degree polynomials in the coarse meshes. By this way, it is possible to relax the CFL condition and in the same time, the dispersion effects are limited. Unfortunately, the cell-size variations are so important that this strategy is not sufficient. One solution could be to apply implicit and unconditionally stable schemes, which would obviously free us from the CFL constraint. Unfortunately, these schemes require inverting a linear system at each iteration and thus needs huge computational burden that can be prohibitive in 3D. Moreover, numerical dispersion may be increased. Then, as second solution is the use of local time stepping strategies for matching the time step to the different sizes of the mesh. There are several attempts [66], [63], [79], [75], [68] and Magique 3D has proposed a new time stepping method which allows us to adapt both the time step and the order of time approximation to the size of the cells. Nevertheless, despite a very good performance assessment in academic configurations, we have observed to our detriment that its implementation inside industrial codes is not obvious and in practice, improvements of the computational costs are disappointing, especially in a HPC framework. Indeed, the local time stepping algorithm may strongly affect the scalability of the code. Moreover, the complexity of the algorithm is increased when dealing with lossy media [71].

Recently, Dolean *et al* [67] have considered a novel approach consisting in applying hybrid schemes combining second order implicit schemes in the thin cells and second order explicit discretization in the coarse mesh. Their numerical results indicate that this method could be a good alternative but the numerical dispersion is still present. It would then be interesting to implement this idea with high-order time schemes to reduce the numerical dispersion. The recent arrival in the team of J. Chabassier should help us to address this problem since she has the expertise in constructing high-order implicit time scheme based on energy preserving Newmark schemes [64]. We propose that our work be organized around the two following tasks. The first one is the extension of these schemes to the case of lossy media because applying existing schemes when there is attenuation is not straightforward. This is a key issue because there is artificial attenuation when absorbing boundary conditions are introduced and if not, there are cases with natural attenuation like in visco-elastic media. The second one is the coupling of high-order implicit schemes with high-order explicit schemes. These two tasks can be first completed independently, but the ultimate goal is obviously to couple the schemes for lossy media. We will consider two strategies for the coupling. The first one will be based on the method proposed by Dolean *et al*, the second one will consist in using Lagrange multiplier on the interface between the coarse and fine grids and write a novel coupling condition that ensures the high order consistency of the global scheme. Besides these theoretical aspects, we will have to implement the method in industrial codes and our discretization methodology is very suitable for parallel computing since it involves Lagrange multipliers. We propose to organize this task as follows. There is first the crucial issue of a systematic distribution of the cells in the coarse/explicit and in the fine/implicit part. Based on our experience on local time stepping, we claim that it is necessary to define a criterion which discriminates thin cells from coarse ones. Indeed, we intend to develop codes which will be used by practitioners, in particular engineers working in the production department of Total. It implies that the code will be used by people who are not necessarily experts in scientific computing. Considering real-world problems means that the mesh will most probably be composed of a more or less high number of subsets arbitrarily distributed and containing thin or coarse cells. Moreover, in the prospect of solving inverse problems, it is difficult to assess which cells are thin or not in a mesh which varies at each iteration.

Another important issue is the load balancing that we can not avoid with parallel computing. In particular, we will have to choose one of these two alternatives: dedicate one part of processors to the implicit computations and the other one to explicit calculus or distribute the resolution with both schemes on all processors. A collaboration with experts in HPC is then mandatory since we are not expert in parallel computing. We will thus continue to collaborate with the team-projects Hiepacs and Runtime with whom we have a long-term experience of collaborations. The load-balancing leads then to the issue of mesh partitioning. Main mesh partitioners are very efficient for the coupling of different discretizations in space but to the best of our knowledge, the case of non-uniform time discretization has never been addressed. The study of meshes being out of the scopes of Magique-3D, we will collaborate with experts on mesh partitioning. We get already on to François Pellegrini who is the principal investigator of Scotch (http://www.labri.fr/perso/pelegrin/scotch) and permanent member of the team project Bacchus (Inria Bordeaux Sud Ouest Research Center).

In the future, we aim at enlarging the application range of implicit schemes. The idea will be to use the degrees of freedom offered by the implicit discretization in order to tackle specific difficulties that may appear in some systems. For instance, in systems involving several waves (as P and S waves in porous elastic media, or coupled wave problems as previously mentioned) the implicit parameter could be adapted to each wave and optimized in order to reduce the computational cost. More generally, we aim at reducing numeric bottlenecks by adapting the implicit discretization to specific cases.

MAMBA Project-Team

3. Research Program

3.1. Introduction

At small spatial scales, or at spatial scales of individual matter components, where heterogeneities in the medium occur, agent-based models are developed ([0], [76], Dirk Drasdo's former associate team QUANTISS). Another approach, that is considered in the project-team MAMBA consists in considering gene expression at the individual level by stochastic processes [0], by ordinary differential equations [0], or by a mixed representation of Markov processes and ordinary differential equations [0], the outputs of which quantify focused aspects of biological variability in a population of individuals (cells) under study.

Both these approaches complement the partial differential equation models considered on scales at which averages over the individual components behave sufficiently smoothly. Investigating the links between these models through scales is also part of our research [0]. Moreover, in order to quantitatively assess the adequacy between the biological phenomena we study and the mathematical models we use, we also develop inverse problem methods.

3.2. PDE analysis and simulation

PDEs arise at several levels of our models. Parabolic equations [0] can be used for large cell populations and also for intracellular spatio-temporal dynamics of proteins and their messenger RNAs in gene regulatory networks, transport equations [0] are used for protein aggregation / fragmentation models and for the cell division cycle in age-structured models of proliferating cell populations. Existence, uniqueness and asymptotic behaviour of solutions have been studied [65], [62]. Other equations, of the integro-differential type, dedicated to describing the Darwinian evolution of a cell population according to a phenotypic trait, allowing exchanges with the environment, genetic mutations and reversible epigenetic modifications, are also used [81], [80], [79], [82], possibly enriched to classical PDEs by the adjunction of diffusion and advection terms [63]. Through multiscale analysis, they can be related to stochastic and free boundary models used in cancer modelling.

3.3. Inverse problems

When studying biological populations (usually cells or big molecules) using PDE models, identification of the functions and parameters that govern the dynamics of a model may be achieved to a certain extent by statistics performed on individuals to reconstruct the probability distribution of their relevant characteristics in the population they constitute, but quantitative observations at the individual level (e.g., fluorescence in single cells [60] or size/age tracking [87]) require sophisticated techniques and are most often difficult to obtain. Relying on the accuracy of a PDE model to describe the population dynamics, inverse problem methods offer a tractable alternative in model identification, and they are presently an active theme of research in MAMBA. Following previous studies [68], [69], some combining statistical and deterministic approaches [67] with application to raw experimental data [66], we plan to develop our methods to new structured-population models (or stochastic fragmentation processes as in [66]), useful for other types of data or populations (e.g. size/age tracking, polymer length distribution, fluorescence in single cells).

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3.4. Stochastic and agent-based models

The link between stochastic processes and kinetic equations is a domain already present in our research [0] [67] and that we plan to develop further. They can be viewed either as complementary approaches, useful to take into account different scales (smaller scales for stochastic models, larger scales for mean-field limits), or even as two different viewpoints on the same problem [66], enriching each other. Neuroscience is a domain where this is particularly true because noise contributes significantly to the activity of neurons; this is the case of networks where mean field limits are derived from stochastic individual-based models and lead to fundamental questions on the well-posedness and behaviours of the system [0]. One strength and originality of our project is our close connection and collaboration not only with probability theorists but also with statisticians, who provide us with efficient help in the identification of our model parameters.

Agent-based systems consider each component individually. For example, in multi-cellular system modelling, the basic unit is the cell, and each cell is considered [70], [89]. This approach has advantages if the population of cells reveals heterogeneities on small spatial scales as it occurs if organ architecture is represented [76], or if the number of cells in a particular state is small. Different approaches have been used to model cellular agents in multi-cellular systems in space, roughly divided in lattice models (e.g. [85]) and in lattice-free (or off-lattice) models, in which the position [70], [73] or even the shape (e.g. [89]) of the cell can change gradually.

The dynamics of cells in lattice-based models is usually described by rules chosen to mimic the behaviour of a cell including its physical behavior. The advantage of this approach is that it is simpler and that simulation times for a given number of cells are shorter than in lattice-free models. In contrast, most lattice-free models attempt to parameterise cells by measurable values with a direct physical or biological meaning, hence allowing identification of physiologically meaningful parameter ranges. This improves model simulation feasibility, since parameter sensitivity analyses in simulations shows significant improvements when a high dimensional parameter space can be reduced. It also facilitates the development of systematic systems biology and systems medicine strategies to identify mechanisms underlying complex tissue organisation processes ([89], [71]).

Moreover, it is straightforward to include relevant signal transduction and metabolic pathways in each cell within the framework of agent-based models, which is a key advantage in the present times, as the interplay of components at many levels is more and more precisely studied [91].

3.5. Multi-level modelling

Multi-level modelling addresses models spanning many spatial scales composed of functional connected modules on each of these scales [64]. Typical representatives of multilevel systems are organs, that are composed of cells of different types coordinated in space, extracellular matrix, etc. Development, parameterisation, verification and validation of such models is challenging as it is usually not possible to simultaneously perform experimental measurements on each level simultaneously.

The fundamental strategy is composed of a multi-step strategy, parameterising sub-models individually before connecting them [71]. For this, models shall be parameterised by measurable quantities for which parameter ranges can be reliably estimated. Then simulated parameter sensitivity simulations are run, comparing results with experiments. If the best agreement between model and experiment is insufficient, the model is wrong or incomplete. If several models are able to explain the data, settings should be run with these models that lead to experimentally testable distinguishable outcomes.

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MATHNEURO Team

3. Research Program

3.1. Neural networks dynamics

The study of neural networks is certainly motivated by the long term goal to understand how brain is working. But, beyond the comprehension of brain or even of simpler neural systems in less evolved animals, there is also the desire to exhibit general mechanisms or principles at work in the nervous system. One possible strategy is to propose mathematical models of neural activity, at different space and time scales, depending on the type of phenomena under consideration. However, beyond the mere proposal of new models, which can rapidly result in a plethora, there is also a need to understand some fundamental keys ruling the behaviour of neural networks, and, from this, to extract new ideas that can be tested in real experiments. Therefore, there is a need to make a thorough analysis of these models. An efficient approach, developed in our team, consists of analysing neural networks as dynamical systems. This allows to address several issues. A first, natural issue is to ask about the (generic) dynamics exhibited by the system when control parameters vary. This naturally leads to analyse the bifurcations [8] [37] occurring in the network and which phenomenological parameters control these bifurcations. Another issue concerns the interplay between neuron dynamics and synaptic network structure.

3.2. Mean-field approaches

Modeling neural activity at scales integrating the effect of thousands of neurons is of central importance for several reasons. First, most imaging techniques are not able to measure individual neuron activity (microscopic scale), but are instead measuring mesoscopic effects resulting from the activity of several hundreds to several hundreds of thousands of neurons. Second, anatomical data recorded in the cortex reveal the existence of structures, such as the cortical columns, with a diameter of about $50\mu m$ to $1mm$, containing of the order of one hundred to one hundred thousand neurons belonging to a few different species. The description of this collective dynamics requires models which are different from individual neurons models. In particular, when the number of neurons is large enough averaging effects appear, and the collective dynamics is well described by an effective mean-field, summarizing the effect of the interactions of a neuron with the other neurons, and depending on a few effective control parameters. This vision, inherited from statistical physics requires that the space scale be large enough to include a large number of microscopic components (here neurons) and small enough so that the region considered is homogeneous.

Our group is developing mathematical and numerical methods allowing on one hand to produce dynamic mean-field equations [1] [36] from the physiological characteristics of neural structure (neurons type, synapse type and anatomical connectivity between neurons populations), and on the other so simulate these equations.

3.3. Neural fields

Neural fields are a phenomenological way of describing the activity of population of neurons by delay integro-differential equations. This continuous approximation turns out to be very useful to model large brain areas such as those involved in visual perception. The mathematical properties of these equations and their solutions are still imperfectly known, in particular in the presence of delays, different time scales and of noise.

Our group is developing mathematical and numerical methods for analysing these equations. These methods are based upon techniques from mathematical functional analysis, bifurcation theory [9], equivariant bifurcation analysis, delay equations, and stochastic partial differential equations. We have been able to characterize the solutions of these neural fields equations and their bifurcations, apply and expand the theory to account for such perceptual phenomena as edge, texture [3], and motion perception. We have also developed a theory of the delayed neural fields equations, in particular in the case of constant delays and propagation delays that must be taken into account when attempting to model large size cortical areas [38]. This theory is based on center manifold and normal forms ideas.

3.4. Slow-Fast Dynamics in Neuronal Models

Neuronal rhythms typically display many different timescales, therefore it is important to incorporate this slow-fast aspect in models. We are interested in this modeling paradigm where slow-fast point models (using Ordinary Differential Equations) are investigated in terms of their bifurcation structure and the patterns of oscillatory solutions that they can produce. To insight into the dynamics of such systems, we use a mix of theoretical techniques — such as geometric desingularisation and centre manifold reduction [35] — and numerical methods such as pseudo-arclength continuation [32]. We are interested in families of complex oscillations generated by both mathematical and biophysical models of neurons. In particular, so-called *mixed-mode oscillations (MMOs) [30], [34])*, which represent an alternation between subthreshold and spiking behaviour, and *bursting oscillations* [31], [33], also corresponding to experimentally observed behaviour [29].

Selected publications on this topic: lien.

3.5. Synaptic Plasticity

Neural networks show amazing abilities to evolve and adapt, and to store and process information. These capabilities are mainly conditioned by plasticity mechanisms, and especially synaptic plasticity, inducing a mutual coupling between network structure and neuron dynamics. Synaptic plasticity occurs at many levels of organization and time scales in the nervous system [28]. It is of course involved in memory and learning mechanisms, but it also alters excitability of brain areas and regulates behavioral states (e.g. transition between sleep and wakeful activity). Therefore, understanding the effects of synaptic plasticity on neurons dynamics is a crucial challenge.

Our group is developing mathematical and numerical methods to analyse this mutual interaction. On the one hand, we have shown that plasticity mechanisms, Hebbian-like or STDP, have strong effects on neuron dynamics complexity, such as dynamics complexity reduction, and spike statistics

3.6. Visual Neuroscience

Our group focuses on the visual system to understand how information is encoded and processed resulting in visual percepts. To do so, we propose functional models of the visual system using a variety of mathematical formalisms, depending on the scale at which models are built, such as spiking neural networks or neural fields. So far, our efforts have been focused on the study of retinal processing, edge and texture perception, motion integration at the level of V1 and MT cortical areas.

MIMESIS Team

3. Research Program

3.1. Modeling of complex anatomical environments

Objectives:

- Coupled and multi-physics models & Non-linear and composite models
- Smooth and high-order FEM
- Hierarchical and heterogeneous representations

Milestones:

- Composite structures (e.g. vascularized organs)
- Integration of hyper-elastic materials and higher-order elements
- Combined behaviors (e.g. electro-mechanical model of the heart)

A central objective of this challenge is the modeling of the biomechanics and physiology of organs under various stimuli. This requires to describe different biophysical phenomena such as soft-tissue deformation, fluid dynamics, electrical propagation, or heat transfer. These models will help simulate the impact of different therapies (such as cryosurgery, radio-frequency ablation, surgical resection), but also represent the behavior of complex organs such as the brain, the liver or the heart (Figure 2).

A common requirement across these developments is the need for (near) real-time computation and the ability to adapt to patient-specific characteristics. Simulating such complex surgical environments involves the coupled use of composite models coming with their own discretizations that differ in terms of topology and dimension. This requires methods involving hierarchical or multi-resolution models that provide an inherent solution for the coupling of such heterogeneous representations. Another, related, objective is to study methods able to locally adapt the mesh resolution (when using an FEM approach) to the need of the simulation or to simulate the propagation of fractures during soft tissue tearing.

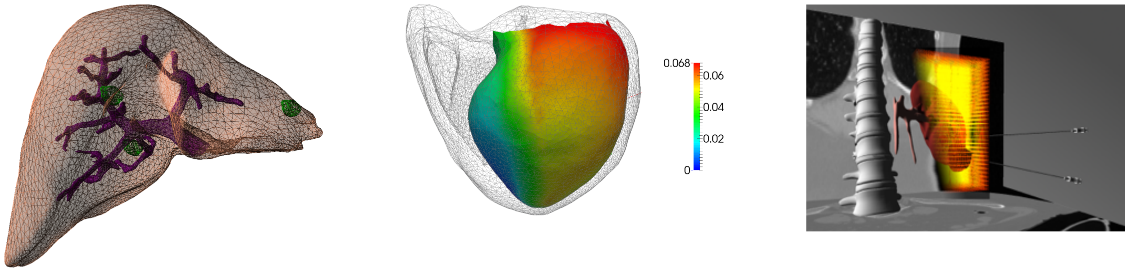

Figure 2. Left: patient-specific liver model with its vascular system. Middle: patient specific depolarization times. Right: cryoablation in the kidney.

An important part of our research is dedicated to the development of new accurate models that remain compatible with real-time computation. Such advanced models not only permit to increase the realism of future training systems, but also act as a bridge toward the development of patient-specific preoperative planning as well as augmented reality tools for the operating room. Yet, patient-specific planning or per-operative guidance also requires the models to be parametrized with patient-specific biomechanical data. The objective in this area is related to the study of hyper-elastic models and their validation for a range of tissues. Preliminary work in this area has been done through two collaborations, one with the biomechanical lab in Lille (LML), and the biomechanics group from the ICube laboratory in Strasbourg on the development and validation of liver and kidney models.

Another important research topic will be related to model reduction through various approaches, such as Proper Generalized Decomposition (PGD) or modal analysis. We are currently collaborationg with the Legato team at University of Luxembourg which has good expertise in this area. Similar approaches, such as the use of Krylov spaces, have already been studied in our group recently.

We are transitioning from our work on cardiac electro-physiology simulation to the modeling of the electrical conduction in soft tissues as well as optimization problems in the context of heat diffusion. This is a key element of the development of both planning and guidance systems for percutaneous procedures, such that an optimal therapeutical effect can be reached.

3.2. Numerical methods for real-time simulation

Objectives:

- Numerical solution of systems of equations
- Acceleration and optimization with parallel computing
- Context-aware discretization and adaptive (re)meshing for cuts and fractures
- Advanced constraints: Interaction, multi-body contacts - Collision detection

Milestones:

- Simulation of cutting, fracture and tearing
- Finite element simulation using adaptive meshing
- Mixed or hybrid finite element methods

The principal objective of this second challenge is to improve, at the numerical level, the efficiency, robustness, and quality of the simulations. To reach these goals, we essentially rely on two approaches: **adaptive meshing** to allow mesh transformations during a simulation and support cuts, local remeshing or dynamic refinement in areas of interest; and **numerical techniques**, such as asynchronous solvers, domain decomposition and model order reduction (Figure 3).

Typically, the simulations in the field of biomechanics, physiological modeling, or even computer graphics, employ techniques based on the finite element method. Such simulations require a discretization of the domain of interest, and this discretization is traditionally made of tetrahedral or hexahedral elements. The topology defined by these elements is also considered constant. The first objective of this work is to jointly develop advanced topological operations and new finite element approaches that can leverage the use of dynamic topologies. In particular we focus our research on multi-resolution meshes where elements are subdivided in areas where numerical errors need to be kept small [25], [27].

Once the problem, as defined in the previous challenge, has been discretized, we need to solve a large system of linear or nonlinear equations. In both cases, it is necessary to employ numerical solvers repeatedly to construct the solution representing the state of the simulated system. In the past years, we have contributed to this topic through our work on asynchronous preconditioning [19]. We would like to pursue this area of research exploiting the relevant advances in hierarchy-based topologies (e.g. the multi-grid methods). We will also consider advanced non-linear solvers which are necessary for correct resolution of hyper-elastic models and composite models.

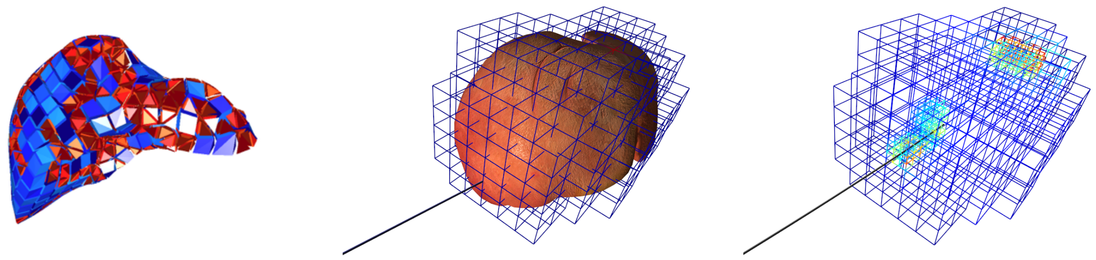

Figure 3. Left: Patient-specific mixed (tetrahedral + hexahedral) mesh of the liver. Middle: liver surface embedded into an hexahedral mesh. Right: dynamic subdivision of the mesh based on geometrical and mechanical constraints.

Finally, to improve computational times from a programming stand-point, we have started a collaboration with the CAMUS team at Inria. This collaboration aims at using smart code analysis and on-the-fly parallelism to automatically speed-up computation times. In a typical scenario, the modeled organ or tissue is surrounded by its environment represented by other organs, connective tissues or fat. Further, during the intervention, the tissues are manipulated with instruments. Therefore, the interaction will also be an important aspect of our research. We have already developed methods for modeling of advanced interactions between organs, tissues and tools [24] [20]. We will continue exploiting novel methods such as partial factorization [28] and integrate our approach with other techniques such as augmented Lagrangian.

3.3. Data-driven simulation

Objectives:

- Stochastic filtering
- Inverse modeling
- Parametrization and estimation of the boundary conditions
- Validation and experimental assessment

Milestones:

- Non-rigid registration using biomechanical models
- Augmented reality for hepatic surgery
- 3D-2D real-time fusion for vascular surgery

Image-guided simulation has been a recent area of research in our team. We believe it has the potential to bridge the gap between medical imaging and clinical routine by adapting pre-operative data to the time of the procedure. Several challenges are related to image-guided therapy but the main issue consists in aligning pre-operative images onto the patient and keep this alignment up-to-date during the procedure. As most procedures deal with soft-tissues, elastic registration techniques are necessary to perform this step.

Recently, registration techniques started to account for soft tissue biomechanics using physically-based methods, yet several limitations still hinder the use of image-guided therapy in clinical routine. First, as registration methods become more complex, their computation times increase, thus lacking responsiveness. Second, techniques used for non-rigid registration or deformable augmented reality only “borrow” ideas from continuum mechanics but lack some key elements (such as identification of the rest shape, or definition of the boundary conditions). Also, these registration or augmented reality problems are highly dependent on the choice of image modality and require to investigate some aspects of computer vision or medical image processing. However, if we can properly address these challenges, the combination of a real-time simulation and regular acquisitions of image data during the procedure opens up very interesting possibilities by using data assimilation to better adapt the model to intra-operative data, not limited to image-based information.

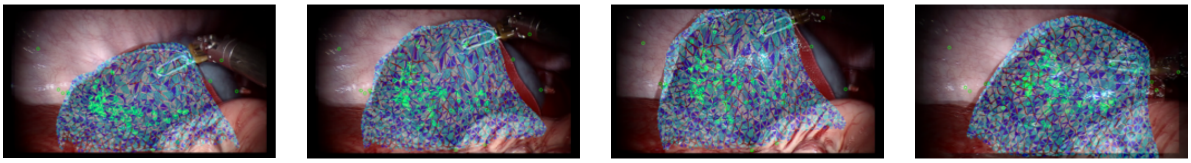

Figure 4. Real-time deformation of a virtual liver according to tissue motion tracked in laparoscopic images.

In the area of non-rigid registration and augmented reality, we have already demonstrated the benefit of our physics-based approaches. This was applied in particular to the problem of organ tracking during surgery (Figure 4) and led to several key publications [22] [23] [21] and awards (best paper ISMAR 2013, second best paper at IPCAI 2014). We continue this work with an emphasis on robustness to uncertainty and outliers in the information extracted in real-time from image data and by improving upon our current computer vision techniques, in particular to guarantee a very accurate initial registration of the pre-operative model onto the per-operative surface patch extracted from monocular or stereo laparoscopic cameras. This work will finally benefit from advances in the challenges listed previously, in particular real-time hyper-elastic models of behavior.

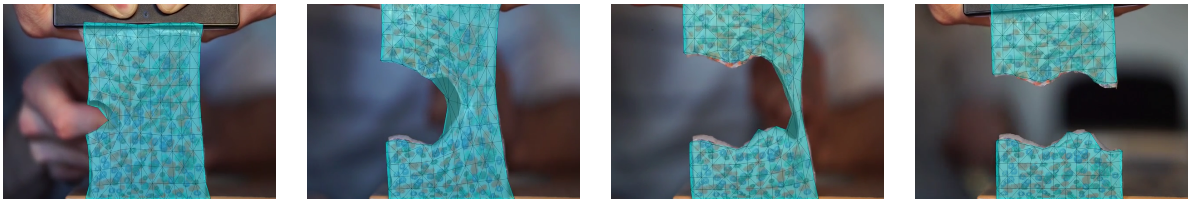

Figure 5. An augmented elastic object is torn. The cut is detected and applied to the virtual model in real time.

The use of simulation in the context of image-guided therapy can be extended in several other ways. A direction we are addressing is the combined use of simulation and X-ray imaging during interventional radiology procedures. Whether it is for percutaneous procedures or catheterization, the task of the simulation is to provide a short-term (1 to 5 seconds) prediction of the needle or catheter position. Using information extracted from the image, the parameters of the simulation can be assimilated (using methods such as unscented Kalman filters), so that the simulation progressively matches the real data in order to reduce uncertainties. We have already started to create a flexible framework integrating the real-time soft-tissue simulation and state-of-the-art methods of data assimilation and filtering.

MNEMOSYNE Project-Team

3. Research Program

3.1. Integrative and Cognitive Neuroscience

The human brain is often considered as the most complex system dedicated to information processing. This multi-scale complexity, described from the metabolic to the network level, is particularly studied in integrative neuroscience, the goal of which is to explain how cognitive functions (ranging from sensorimotor coordination to executive functions) emerge from (are the result of the interaction of) distributed and adaptive computations of processing units, displayed along neural structures and information flows. Indeed, beyond the astounding complexity reported in physiological studies, integrative neuroscience aims at extracting, in simplifying models, regularities at various levels of description. From a mesoscopic point of view, most neuronal structures (and particularly some of primary importance like the cortex, cerebellum, striatum, hippocampus) can be described through a regular organization of information flows and homogenous learning rules, whatever the nature of the processed information. From a macroscopic point of view, the arrangement in space of neuronal structures within the cerebral architecture also obeys a functional logic, the sketch of which is captured in models describing the main information flows in the brain, the corresponding loops built in interaction with the external and internal (bodily and hormonal) world and the developmental steps leading to the acquisition of elementary sensorimotor skills up to the most complex executive functions.

In summary, integrative neuroscience builds, on an overwhelming quantity of data, a simplifying and interpretative grid suggesting homogenous local computations and a structured and logical plan for the development of cognitive functions. They arise from interactions and information exchange between neuronal structures and the external and internal world and also within the network of structures.

This domain is today very active and stimulating because it proposes, of course at the price of simplifications, global views of cerebral functioning and more local hypotheses on the role of subsets of neuronal structures in cognition. In the global approaches, the integration of data from experimental psychology and clinical studies leads to an overview of the brain as a set of interacting memories, each devoted to a specific kind of information processing [54]. It results also in longstanding and very ambitious studies for the design of cognitive architectures aiming at embracing the whole cognition. With the notable exception of works initiated by [50], most of these frameworks (e.g. Soar, ACT-R), though sometimes justified on biological grounds, do not go up to a *connectionist* neuronal implementation. Furthermore, because of the complexity of the resulting frameworks, they are restricted to simple symbolic interfaces with the internal and external world and to (relatively) small-sized internal structures. Our main research objective is undoubtly to build such a general purpose cognitive architecture (to model the brain *as a whole* in a systemic way), using a connectionist implementation and able to cope with a realistic environment.

3.2. Computational Neuroscience

From a general point of view, computational neuroscience can be defined as the development of methods from computer science and applied mathematics, to explore more technically and theoretically the relations between structures and functions in the brain [56], [43]. During the recent years this domain has gained an increasing interest in neuroscience and has become an essential tool for scientific developments in most fields in neuroscience, from the molecule to the system. In this view, all the objectives of our team can be described as possible progresses in computational neuroscience. Accordingly, it can be underlined that the systemic view that we promote can offer original contributions in the sense that, whereas most classical models in computational neuroscience focus on the better understanding of the structure/function relationship for isolated specific structures, we aim at exploring synergies between structures. Consequently, we target interfaces and interplay between heterogenous modes of computing, which is rarely addressed in classical computational neuroscience.

We also insist on another aspect of computational neuroscience which is, in our opinion, at the core of the involvement of computer scientists and mathematicians in the domain and on which we think we could particularly contribute. Indeed, we think that our primary abilities in numerical sciences imply that our developments are characterized above all by the effectiveness of the corresponding computations: We provide biologically inspired architectures with effective computational properties, such as robustness to noise, self-organization, on-line learning. We more generally underline the requirement that our models must also mimick biology through its most general law of homeostasis and self-adaptability in an unknown and changing environment. This means that we propose to numerically experiment such models and thus provide effective methods to falsify them.

Here, computational neuroscience means mimicking original computations made by the neuronal substratum and mastering their corresponding properties: computations are distributed and adaptive; they are performed without an homonculus or any central clock. Numerical schemes developed for distributed dynamical systems and algorithms elaborated for distributed computations are of central interest here [40], [49] and were the basis for several contributions in our group [55], [52], [57]. Ensuring such a rigor in the computations associated to our systemic and large scale approach is of central importance.

Equally important is the choice for the formalism of computation, extensively discussed in the connectionist domain. Spiking neurons are today widely recognized of central interest to study synchronization mechanisms and neuronal coupling at the microscopic level [41]; the associated formalism [46] can be possibly considered for local studies or for relating our results with this important domain in connectionism. Nevertheless, we remain mainly at the mesoscopic level of modeling, the level of the neuronal population, and consequently interested in the formalism developed for dynamic neural fields [38], that demonstrated a richness of behavior [42] adapted to the kind of phenomena we wish to manipulate at this level of description. Our group has a long experience in the study and adaptation of the properties of neural fields [52], [53] and their use for observing the emergence of typical cortical properties [45]. In the envisioned development of more complex architectures and interplay between structures, the exploration of mathematical properties such as stability and boundedness and the observation of emerging phenomena is one important objective. This objective is also associated with that of capitalizing our experience and promoting good practices in our software production (*cf.* § 6.1). In summary, we think that this systemic approach also brings to computational neuroscience new case studies where heterogenous and adaptive models with various time scales and parameters have to be considered jointly to obtain a mastered substratum of computation. This is particularly critical for large scale deployments, as we will discuss in § 6.1).

3.3. Machine Learning

The adaptive properties of the nervous system are certainly among its most fascinating characteristics, with a high impact on our cognitive functions. Accordingly, machine learning is a domain [48] that aims at giving such characteristics to artificial systems, using a mathematical framework (probabilities, statistics, data analysis, etc.). Some of its most famous algorithms are directly inspired from neuroscience, at different levels. Connectionist learning algorithms implement, in various neuronal architectures, weight update rules, generally derived from the hebbian rule, performing non supervised (e.g. Kohonen self-organizing maps), supervised (e.g. layered perceptrons) or associative (e.g. Hopfield recurrent network) learning. Other algorithms, not necessarily connectionist, perform other kinds of learning, like reinforcement learning. Machine learning is a very mature domain today and all these algorithms have been extensively studied, at both the theoretical and practical levels, with much success. They have also been related to many functions (in the living and artificial domains) like discrimination, categorisation, sensorimotor coordination, planning, etc. and several neuronal structures have been proposed as the substratum for these kinds of learning [44], [37]. Nevertheless, we believe that, as for previous models, machine learning algorithms remain isolated tools, whereas our systemic approach can bring original views on these problems.

At the cognitive level, most of the problems we face do not rely on only one kind of learning and require instead skills that have to be learned in preliminary steps. That is the reason why cognitive architectures are often referred to as systems of memory, communicating and sharing information for problem solving. Instead of the classical view in machine learning of a flat architecture, a more complex network of modules must be considered here, as it is the case in the domain of deep learning. In addition, our systemic approach brings the question of incrementally building such a system, with a clear inspiration from developmental sciences. In this perspective, modules can generate internal signals corresponding to internal goals, predictions, error signals, able to supervise the learning of other modules (possibly endowed with a different learning rule), supposed to become autonomous after an instructing period. A typical example is that of episodic learning (in the hippocampus), storing declarative memory about a collection of past episods and supervising the training of a procedural memory in the cortex.

At the behavioral level, as mentionned above, our systemic approach underlines the fundamental links between the adaptive system and the internal and external world. The internal world includes proprioception and interoception, giving information about the body and its needs for integrity and other fundamental programs. The external world includes physical laws that have to be learned and possibly intelligent agents for more complex interactions. Both involve sensors and actuators that are the interfaces with these worlds and close the loops. Within this rich picture, machine learning generally selects one situation that defines useful sensors and actuators and a corpus with properly segmented data and time, and builds a specific architecture and its corresponding criteria to be satisfied. In our approach however, the first question to be raised is to discover what is the goal, where attention must be focused on and which previous skills must be exploited, with the help of a dynamic architecture and possibly other partners. In this domain, the behavioral and the developmental sciences, observing how and along which stages an agent learns, are of great help to bring some structure to this high dimensional problem.

At the implementation level, this analysis opens many fundamental challenges, hardly considered in machine learning : stability must be preserved despite on-line continuous learning; criteria to be satisfied often refer to behavioral and global measurements but they must be translated to control the local circuit level; in an incremental or developmental approach, how will the development of new functions preserve the integrity and stability of others? In addition, this continous re-arrangement is supposed to involve several kinds of learning, at different time scales (from msec to years in humans) and to interfer with other phenomena like variability and meta-plasticity.

In summary, our main objective in machine learning is to propose on-line learning systems, where several modes of learning have to collaborate and where the protocoles of training are realistic. We promote here a *really autonomous* learning, where the agent must select by itself internal resources (and build them if not available) to evolve at the best in an unknown world, without the help of any *deus-ex-machina* to define parameters, build corpus and define training sessions, as it is generally the case in machine learning. To that end, autonomous robotics (*cf.* § 3.4) is a perfect testbed.

3.4. Autonomous Robotics

Autonomous robots are not only convenient platforms to implement our algorithms; the choice of such platforms is also motivated by theories in cognitive science and neuroscience indicating that cognition emerges from interactions of the body in direct loops with the world (*embodiment of cognition* [39]). In addition to real robotic platforms, software implementations of autonomous robotic systems including components dedicated to their body and their environment will be also possibly exploited, considering that they are also a tool for studying conditions for a real autonomous learning.

A real autonomy can be obtained only if the robot is able to define its goal by itself, without the specification of any high level and abstract cost function or rewarding state. To ensure such a capability, we propose to endow the robot with an artificial physiology, corresponding to perceive some kind of pain and pleasure. It may consequently discriminate internal and external goals (or situations to be avoided). This will mimick circuits related to fundamental needs (e.g. hunger and thirst) and to the preservation of bodily integrity. An important objective is to show that more abstract planning capabilities can arise from these basic goals.

A real autonomy with an on-line continuous learning as described in § 3.3 will be made possible by the elaboration of protocols of learning, as it is the case, in animal conditioning, for experimental studies where performance on a task can be obtained only after a shaping in increasingly complex tasks. Similarly, developmental sciences can teach us about the ordered elaboration of skills and their association in more complex schemes. An important challenge here is to translate these hints at the level of the cerebral architecture.

As a whole, autonomous robotics permits to assess the consistency of our models in realistic condition of use and offers to our colleagues in behavioral sciences an object of study and comparison, regarding behavioral dynamics emerging from interactions with the environment, also observable at the neuronal level.

In summary, our main contribution in autonomous robotics is to make autonomy possible, by various means corresponding to endow robots with an artificial physiology, to give instructions in a natural and incremental way and to prioritize the synergy between reactive and robust schemes over complex planning structures.

MONC Project-Team

3. Research Program

3.1. Introduction

Our research on mathematical oncology is three-fold:

- Axis 1: Tumor modeling for patient-specific simulations.
- Axis 2: Bio-physical modeling for personalized therapies.
- Axis 3: Quantitative cancer modeling for biological and preclinical studies.

In the first axis, we aim at producing patient-specific simulations of the growth of a tumor or its response to treatment starting from a series of images. We hope to be able to offer a valuable insight on the disease to the clinicians in order to improve the decision process. This would be particularly useful in the cases of relapses or for metastatic diseases.

The second axis aims at modeling biophysical therapies like radiotherapies, but also thermo-ablations, radio-frequency ablations or electroporation that play a crucial role in the case of a relapse or for a metastatic disease, which is precisely the clinical context where the techniques of axis 1 will be applied.

The third axis, even if not directly linked to clinical perspectives, is essential since it is a way to better understand and model the biological reality of cancer growth and the (possibly complex) effects of therapeutic intervention. Modeling in this case also helps to interpret the experimental results and improve the accuracy of the models used in Axis 1. Technically speaking, some of the computing tools are similar to those of Axis 1.

3.2. Axis 1: Tumor modeling for patient-specific simulations

The gold standard treatment for most cancers is surgery. In the case where total resection of the tumor is possible, the patient often benefits from an adjuvant therapy (radiotherapy, chemotherapy, targeted therapy or a combination of them) in order to eliminate the potentially remaining cells that may not be visible. In this case personalized modeling of tumor growth is useless and statistical modeling will be able to quantify the risk of relapse, the mean progression-free survival time...However if total resection is not possible or if metastases emerge from distant sites, clinicians will try to control the disease for as long as possible. A wide set of tools are available. Clinicians may treat the disease by physical interventions (radiofrequency ablation, cryoablation, radiotherapy, electroporation, focalized ultrasound,...) or chemical agents (chemotherapies, targeted therapies, antiangiogenic drugs, immunotherapies, hormonotherapies). One can also decide to monitor the patient without any treatment (this is the case for slowly growing tumors like some metastases to the lung, some lymphomas or for some low grade glioma). A reliable patient-specific model of tumor evolution with or without therapy may have different uses:

- Case without treatment: the evaluation of the growth of the tumor would offer a useful indication for the time at which the tumor will reach a critical size. For example, radiofrequency ablation of pulmonary lesion is very efficient as long as the diameter of the lesion is smaller than 3 cm. Thus, the prediction can help the clinician plan the intervention. For slowly growing tumors, quantitative modeling can also help to decide at what time interval the patient has to undergo a CT-scan. CT-scans are irradiative exams and there is a challenge for decreasing their occurrence for each patient. It has also an economical impact. And if the disease evolution starts to differ from the forecast, this might mean that some events have occurred at the biological level. For instance, it could be the rise of an aggressive phenotype or cells that leave a dormancy state. This kind of events cannot be predicted, but some mismatch with respect to the prediction can be an indirect proof of their existence. It could be an indication for the clinician to start a treatment.

- Case with treatment: a model can help to understand and to quantify the final outcome of a treatment using the early response. It can help for a redefinition of the treatment planning. Modeling can also help to anticipate the relapse by analyzing some functional aspects of the tumor. Again, a deviation with respect to reference curves can mean a lack of efficiency of the therapy or a relapse. Moreover, for a long time, the response to a treatment has been quantified by the RECIST criteria which consists in (roughly speaking) measuring the diameters of the largest tumor of the patient, as it is seen on a CT-scan. This criteria is still widely used and was quite efficient for chemotherapies and radiotherapies that induce a decrease of the size of the lesion. However, with the systematic use of targeted therapies and anti-angiogenic drugs that modify the physiology of the tumor, the size may remain unchanged even if the drug is efficient and deeply modifies the tumor behavior. One better way to estimate this effect could be to use functional imaging (Pet-scan, perfusion or diffusion MRI, ...), a model can then be used to exploit the data and to understand in what extent the therapy is efficient.
- Optimization: currently, we do not believe that we can optimize a particular treatment in terms of distribution of doses, number, planning with the model that we will develop in a medium term perspective. But it is an aspect that we keep in mind on a long term one.

The scientific challenge is therefore as follows: knowing the history of the patient, the nature of the primitive tumor, its histopathology, knowing the treatments that patients have undergone, knowing some biological facts on the tumor and having a sequence of images (CT-scan, MRI, PET or a mix of them), are we able to provide a numerical simulation of the extension of the tumor and of its metabolism that fits as best as possible with the data (CT-scans or functional data) and that is predictive in order to address the clinical cases described above?

Our approach relies on the elaboration of PDE models and their parametrization with the image by coupling deterministic and stochastic methods. The PDE models rely on the description of the dynamics of cell populations. The number of populations depends on the pathology. For example, for glioblastoma, one needs to use proliferative cells, invasive cells, quiescent cells as well as necrotic tissues to be able to reproduce realistic behaviors of the disease. In order to describe the relapse for hepatic metastases of gastro-intestinal stromal tumor (gist), one needs three cell populations: proliferative cells, healthy tissue and necrotic tissue.

The law of proliferation is often coupled with a model for the angiogenesis. However such models of angiogenesis involve too many non measurable parameters to be used with real clinical data and therefore one has to use simplified or even simplistic versions. The law of proliferation often mimics the existence of an hypoxia threshold, it consists of an O.D.E. or a P.D.E that describes the evolution of the growth rate as a combination of sigmoid functions of nutrients or roughly speaking oxygen concentration. Usually, several laws are available for a given pathology since at this level, there are no quantitative argument to choose a particular one.

The velocity of the tumor growth differs depending on the nature of the tumor. For metastases, we will derive the velocity thanks to Darcy's law in order to express that the extension of the tumor is basically due to the increase of volume. This gives a sharp interface between the metastasis and the surrounding healthy tissues, as observed by anatomopathologists. For primitive tumors like glioma or lung cancer, we use reaction-diffusion equations in order to describe the invasive aspects of such primitive tumors.

The modeling of the drugs depends on the nature of the drug: for chemotherapies, a death term can be added into the equations of the population of cells, while antiangiogenic drugs have to be introduced in a angiogenic model. Resistance to treatment can be described either by several populations of cells or with non-constant growth or death rates. As said before, it is still currently difficult to model the changes of phenotype or mutations, we therefore propose to investigate this kind of phenomena by looking at deviations of the numerical simulations compared to the medical observations.

The calibration of the model is achieved by using a series (at least 2) of images of the same patient and by minimizing a cost function. The cost function contains at least the difference between the volume of the tumor that is measured on the images with the computed one. It also contains elements on the geometry, on the necrosis and any information that can be obtained through the medical images. We will pay special attention to functional imaging (PET, perfusion and diffusion MRI). The inverse problem is solved using a gradient method coupled with some Monte-Carlo type algorithm. If a large number of similar cases is available, one can imagine to use statistical algorithms like random forests to use some non quantitative data like the gender, the age, the origin of the primitive tumor...for example for choosing the model for the growth rate for a patient using this population knowledge (and then to fully adapt the model to the patient by calibrating this particular model on patient data) or for having a better initial estimation of the modeling parameters. We have obtained several preliminary results concerning lung metastases including treatments and for metastases to the liver.

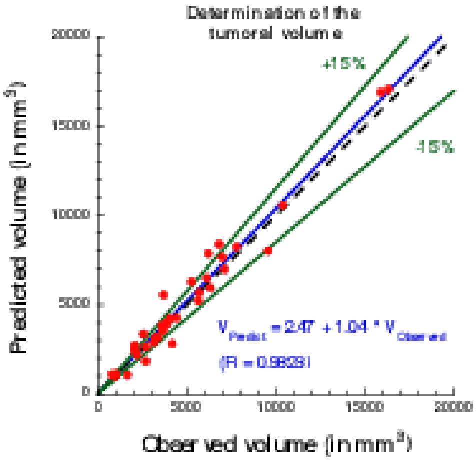

Figure 4. Plot showing the accuracy of our prediction on meningioma volume. Each point corresponds to a patient whose two first exams were used to calibrate our model. A patient-specific prediction was made with this calibrated model and compared with the actual volume as measured on a third time by clinicians. A perfect prediction would be on the black dashed line. Medical data was obtained from Prof. Loiseau, CHU Pellegrin.

3.3. Axis 2: Bio-physical modeling for personalized therapies

In this axis, we investigate locoregional therapies such as radiotherapy, irreversible electroporation. Electroporation consists in increasing the membrane permeability of cells by the delivery of high voltage pulses. This non-thermal phenomenon can be transient (reversible) or irreversible (IRE). IRE or electro-chemotherapy – which is a combination of reversible electroporation with a cytotoxic drug – are essential tools for the treatment of a metastatic disease. Numerical modeling of these therapies is a clear scientific challenge. Clinical applications of the modeling are the main target, which thus drives the scientific approach, even though theoretical studies in order to improve the knowledge of the biological phenomena, in particular for electroporation, should also be addressed. However, this subject is quite wide and we focus on two particular approaches: some aspects of radiotherapies and electro-chemotherapy. This choice is motivated partly by pragmatic reasons: we already have collaborations with physicians on these therapies. Other treatments could be probably treated with the same approach, but we do not plan to work on this subject on a medium term.

- Radiotherapy (RT) is a common therapy for cancer. Typically, using a CT scan of the patient with the structures of interest (tumor, organs at risk) delineated, the clinicians optimize the dose delivery to treat the tumor while preserving healthy tissues. The RT is then delivered every day using low resolution scans (CBCT) to position the beams. Under treatment the patient may lose weight and the tumor shrinks. These changes may affect the propagation of the beams and subsequently change the dose that is effectively delivered. It could be harmful for the patient especially if sensitive organs are concerned. In such cases, a replanification of the RT could be done to adjust the therapeutical protocol. Unfortunately, this process takes too much time to be performed routinely. The challenges faced by clinicians are numerous, we focus on two of them:

  - *Detecting the need of replanification:* we are using the positioning scans to evaluate the movement and deformation of the various structures of interest. Thus we can detect whether or not a structure has moved out of the safe margins (fixed by clinicians) and thus if a replanification may be necessary. In a retrospective study, our work can also be used to determine RT margins when there are no standard ones. A collaboration with the RT department of Institut Bergonié is underway on the treatment of retroperitoneal sarcoma and ENT tumors (head and neck cancers). A retrospective study was performed on 11 patients with retro-peritoneal sarcoma. The results have shown that the safety margins (on the RT) that clinicians are currently using are probably not large enough. The tool used in this study was developed by an engineer funded by Inria (Cynthia Périer, ADT Sesar). We used well validated methods from a level-set approach and segmentation / registration methods. The originality and difficulty lie in the fact that we are dealing with real data in a clinical setup. Clinicians have currently no way to perform complex measurements with their clinical tools. This prevents them from investigating the replanification. Our work and the tools developed pave the way for easier studies on evaluation of RT plans in collaboration with Institut Bergonié. *There was no modeling involved in this work that arose during discussions with our collaborators.* The main purpose of the team is to have meaningful outcomes of our research for clinicians, sometimes it implies leaving a bit our area of expertise.
  - *Evaluating RT efficacy and finding correlation between the radiological responses and the clinical outcome:* our goal is to help doctors to identify correlation between the response to RT (as seen on images) and the longer term clinical outcome of the patient. Typically, we aim at helping them to decide when to plan the next exam after the RT. For patients whose response has been linked to worse prognosis, this exam would have to be planned earlier. This is the subject of collaborations with Institut Bergonié and CHU Bordeaux on different cancers (head and neck, pancreas). The response is evaluated from image markers (*e.g.* using texture information) or with a mathematical model developed in Axis 1. The other challenges are either out of reach or not in the domain of expertise of the team. Yet our works may tackle some important issues for adaptive radiotherapy.

- Both IRE and electrochemotherapy are anticancerous treatments based on the same phenomenon: the electroporation of cell membranes. This phenomenon is known for a few decades but it is still not well understood, therefore our interest is two fold:

  1. We want to use mathematical models in order to better understand the biological behavior and the effect of the treatment. We work in tight collaboration with biologists and bioeletromagneticians to derive precise models of cell and tissue electroporation, in the continuity of the research program of the Inria team-project MC2. These studies lead to complex non-linear mathematical models involving some parameters (as less as possible). Numerical methods to compute precisely such models and the calibration of the parameters with the experimental data are then addressed. Tight collaborations with the Vectorology and Anticancerous Therapies (VAT) of IGR at Villejuif, Laboratoire Ampère of Ecole Centrale Lyon and the Karlsruhe Institute of technology will continue, and we aim at developing new collaborations with Institute of Pharmacology and Structural Biology (IPBS) of Toulouse and the Laboratory of Molecular Pathology and Experimental Oncology (LM-PEO) at CNR Rome, in order to understand differences of the electroporation of healthy cells and cancer cells in spheroids and tissues.

2. This basic research aims at providing new understanding of electroporation, however it is necessary to address, particular questions raised by radio-oncologists that apply such treatments. One crucial question is "What pulse or what train of pulses should I apply to electroporate the tumor if the electrodes are located as given by the medical images"? Even if the real-time optimization of the placement of the electrodes for deep tumors may seem quite utopian since the clinicians face too many medical constraints that cannot be taken into account (like the position of some organs, arteries, nerves...), on can expect to produce real-time information of the validity of the placement done by the clinician. Indeed, once the placement is performed by the radiologists, medical images are usually used to visualize the localization of the electrodes. Using these medical data, a crucial goal is to provide a tool in order to compute in real-time and visualize the electric field and the electroporated region directly on theses medical images, to give the doctors a precise knowledge of the region affected by the electric field. In the long run, this research will benefit from the knowledge of the theoretical electroporation modeling, but it seems important to use the current knowledge of tissue electroporation – even quite rough –, in order to rapidly address the specific difficulty of such a goal (real-time computing of non-linear model, image segmentation and visualization). Tight collaborations with CHU Pellegrin at Bordeaux, and CHU J. Verdier at Bondy are crucial.

- Radiofrequency ablation. In a collaboration with Hopital Haut Leveque, CHU Bordeaux we are trying to determine the efficacy and risk of relapse of hepatocellular carcinoma treated by radiofrequency ablation. For this matter we are using geometrical measurements on images (margins of the RFA, distance to the boundary of the organ) as well as texture information to statistically evaluate the clinical outcome of patients.

3.4. Axis 3: Quantitative cancer modeling for biological and preclinical studies

With the emergence and improvement of a plethora of experimental techniques, the molecular, cellular and tissue biology has operated a shift toward a more quantitative science, in particular in the domain of cancer biology. These quantitative assays generate a large amount of data that call for theoretical formalism in order to better understand and predict the complex phenomena involved. Indeed, due to the huge complexity underlying the development of a cancer disease that involves multiple scales (from the genetic, intra-cellular scale to the scale of the whole organism), and a large number of interacting physiological processes (see the so-called "hallmarks of cancer"), several questions are not fully understood. Among these, we want to focus on the most clinically relevant ones, such as the general laws governing tumor growth and the development of metastases (secondary tumors, responsible of 90% of the deaths from a solid cancer). In this context, it is thus challenging to potentiate the diversity of the data available in experimental settings (such as *in vitro* tumor spheroids or *in vivo* mice experiments) in order to improve our understanding of the disease and its dynamics, which in turn lead to validation, refinement and better tuning of the macroscopic models used in the axes 1 and 2 for clinical applications.

In recent years, several new findings challenged the classical vision of the metastatic development biology, in particular by the discovery of organism-scale phenomena that are amenable to a dynamical description in terms of mathematical models based on differential equations. These include the angiogenesis-mediated distant inhibition of secondary tumors by a primary tumor the pre-metastatic niche or the self-seeding phenomenon Building a general, cancer type specific, comprehensive theory that would integrate these dynamical processes remains an open challenge. On the therapeutic side, recent studies demonstrated that some drugs (such as the Sunitinib), while having a positive effect on the primary tumor (reduction of the growth), could *accelerate* the growth of the metastases. Moreover, this effect was found to be scheduling-dependent. Designing better ways to use this drug in order to control these phenomena is another challenge. In the context of combination therapies, the question of the *sequence* of administration between the two drugs is also particularly relevant.

One of the technical challenge that we need to overcome when dealing with biological data is the presence of potentially very large inter-animal (or inter-individual) variability.

Starting from the available multi-modal data and relevant biological or therapeutic questions, our purpose is to develop adapted mathematical models (*i.e.* identifiable from the data) that recapitulate the existing knowledge and reduce it to its more fundamental components, with two main purposes:

1. to generate quantitative and empirically testable predictions that allow to assess biological hypotheses or
2. to investigate the therapeutic management of the disease and assist preclinical studies of anti-cancerous drug development.

We believe that the feedback loop between theoretical modeling and experimental studies can help to generate new knowledge and improve our predictive abilities for clinical diagnosis, prognosis, and therapeutic decision. Let us note that the first point is in direct link with the axes 1 and 2 of the team since it allows us to experimentally validate the models at the biological scale (*in vitro* and *in vivo* experiments) for further clinical applications.

More precisely, we first base ourselves on a thorough exploration of the biological literature of the biological phenomena we want to model: growth of tumor spheroids, *in vivo* tumor growth in mice, initiation and development of the metastases, effect of anti-cancerous drugs. Then we investigate, using basic statistical tools, the data we dispose, which can range from: spatial distribution of heterogeneous cell population within tumor spheroids, expression of cell makers (such as green fluorescent protein for cancer cells or specific antibodies for other cell types), bioluminescence, direct volume measurement or even intra-vital images obtained with specific imaging devices. According to the data type, we further build dedicated mathematical models that are based either on PDEs (when spatial data is available, or when time evolution of a structured density can be inferred from the data, for instance for a population of tumors) or ODEs (for scalar longitudinal data). These models are confronted to the data by two principal means:

1. when possible, experimental assays can give a direct measurement of some parameters (such as the proliferation rate or the migration speed) or
2. statistical tools to infer the parameters from observables of the model.

This last point is of particular relevance to tackle the problem of the large inter-animal variability and we use adapted statistical tools such as the mixed-effects modeling framework.

Once the models are shown able to describe the data and are properly calibrated, we use them to test or simulate biological hypotheses. Based on our simulations, we then aim at proposing to our biological collaborators new experiments to confirm or infirm newly generated hypotheses, or to test different administration protocols of the drugs. For instance, in a collaboration with the team of the professor Andreas Bikfalvi (Laboratoire de l'Angiogénèse et du Micro-environnement des Cancers, Inserm, Bordeaux), based on confrontation of a mathematical model to multi-modal biological data (total number of cells in the primary and distant sites and MRI), we could demonstrate that the classical view of metastatic dissemination and development (one metastasis is born from one cell) was probably inaccurate, in mice grafted with metastatic kidney tumors. We then proposed that metastatic germs could merge or attract circulating cells. Experiments involving cells tagged with two different colors are currently performed in order to confirm or infirm this hypothesis.

Eventually, we use the large amount of temporal data generated in preclinical experiments for the effect of anti-cancerous drugs in order to design and validate mathematical formalisms translating the biological mechanisms of action of these drugs for application to clinical cases, in direct connection with the axis 1. We have a special focus on targeted therapies (designed to specifically attack the cancer cells while sparing the healthy tissue) such as the Sunitinib. This drug is indeed indicated as a first line treatment for metastatic renal cancer and we plan to conduct a translational study coupled between A. Bikfalvi's laboratory and medical doctors, F. Cornelis (radiologist) and A. Ravaud (head of the medical oncology department).

MORPHEME Project-Team

3. Research Program

3.1. Research Program

The recent advent of an increasing number of new microscopy techniques giving access to high throughput screenings and micro or nano-metric resolutions provides a means for quantitative imaging of biological structures and phenomena. To conduct quantitative biological studies based on these new data, it is necessary to develop non-standard specific tools. This requires using a multi-disciplinary approach. We need biologists to define experiment protocols and interpret the results, but also physicists to model the sensors, computer scientists to develop algorithms and mathematicians to model the resulting information. These different expertises are combined within the Morpheme team. This generates a fecund frame for exchanging expertise, knowledge, leading to an optimal framework for the different tasks (imaging, image analysis, classification, modeling). We thus aim at providing adapted and robust tools required to describe, explain and model fundamental phenomena underlying the morphogenesis of cellular and supra-cellular biological structures. Combining experimental manipulations, in vivo imaging, image processing and computational modeling, we plan to provide methods for the quantitative analysis of the morphological changes that occur during development. This is of key importance as the morphology and topology of mesoscopic structures govern organ and cell function. Alterations in the genetic programs underlying cellular morphogenesis have been linked to a range of pathologies.

Biological questions we will focus on include:

1. what are the parameters and the factors controlling the establishment of ramified structures? (Are they really organize to ensure maximal coverage? How are genetic and physical constraints limiting their morphology?),
2. how are newly generated cells incorporated into reorganizing tissues during development? (is the relative position of cells governed by the lineage they belong to?)

Our goal is to characterize different populations or development conditions based on the shape of cellular and supra-cellular structures, e.g. micro-vascular networks, dendrite/axon networks, tissues from 2D, 2D+t, 3D or 3D+t images (obtained with confocal microscopy, video-microscopy, photon-microscopy or micro-tomography). We plan to extract shapes or quantitative parameters to characterize the morphometric properties of different samples. On the one hand, we will propose numerical and biological models explaining the temporal evolution of the sample, and on the other hand, we will statistically analyze shapes and complex structures to identify relevant markers for classification purposes. This should contribute to a better understanding of the development of normal tissues but also to a characterization at the supra-cellular scale of different pathologies such as Alzheimer, cancer, diabetes, or the Fragile X Syndrome. In this multidisciplinary context, several challenges have to be faced. The expertise of biologists concerning sample generation, as well as optimization of experimental protocols and imaging conditions, is of course crucial. However, the imaging protocols optimized for a qualitative analysis may be sub-optimal for quantitative biology. Second, sample imaging is only a first step, as we need to extract quantitative information. Achieving quantitative imaging remains an open issue in biology, and requires close interactions between biologists, computer scientists and applied mathematicians. On the one hand, experimental and imaging protocols should integrate constraints from the downstream computer-assisted analysis, yielding to a trade-off between qualitative optimized and quantitative optimized protocols. On the other hand, computer analysis should integrate constraints specific to the biological problem, from acquisition to quantitative information extraction. There is therefore a need of specificity for embedding precise biological information for a given task. Besides, a level of generality is also desirable for addressing data from different teams acquired with different protocols and/or sensors. The mathematical modeling of the physics of the acquisition system will yield higher performance reconstruction/restoration algorithms in terms of accuracy. Therefore, physicists and computer scientists have to work together. Quantitative information extraction also has to deal with both the complexity of the structures of interest (e.g., very dense network, small structure detection in a volume, multiscale behavior, ...) and the unavoidable defects of in vivo imaging (artifacts, missing data, ...). Incorporating biological expertise in model-based segmentation methods provides the required specificity while robustness gained from a methodological analysis increases the generality. Finally, beyond image processing, we aim at quantifying and then statistically analyzing shapes and complex structures (e.g., neuronal or vascular networks), static or in evolution, taking into account variability. In this context, learning methods will be developed for determining (dis)similarity measures between two samples or for determining directly a classification rule using discriminative models, generative models, or hybrid models. Besides, some metrics for comparing, classifying and characterizing objects under study are necessary. We will construct such metrics for biological structures such as neuronal or vascular networks. Attention will be paid to computational cost and scalability of the developed algorithms: biological experimentations generally yield huge data sets resulting from high throughput screenings. The research of Morpheme will be developed along the following axes:

- **Imaging:** this includes i) definition of the studied populations (experimental conditions) and preparation of samples, ii) definition of relevant quantitative characteristics and optimized acquisition protocol (staining, imaging, ...) for the specific biological question, and iii) reconstruction/restoration of native data to improve the image readability and interpretation.
- **Feature extraction:** this consists in detecting and delineating the biological structures of interest from images. Embedding biological properties in the algorithms and models is a key issue. Two main challenges are the variability, both in shape and scale, of biological structures and the huge size of data sets. Following features along time will allow to address morphogenesis and structure development.
- **Classification/Interpretation:** considering a database of images containing different populations, we can infer the parameters associated with a given model on each dataset from which the biological structure under study has been extracted. We plan to define classification schemes for characterizing the different populations based either on the model parameters, or on some specific metric between the extracted structures.
- **Modeling:** two aspects will be considered. This first one consists in modeling biological phenomena such as axon growing or network topology in different contexts. One main advantage of our team is the possibility to use the image information for calibrating and/or validating the biological models. Calibration induces parameter inference as a main challenge. The second aspect consists in using a prior based on biological properties for extracting relevant information from images. Here again, combining biology and computer science expertise is a key point.

MYCENAE Project-Team

3. Research Program

3.1. Project team positioning

The main goal of MYCENAE is to address crucial questions arising from both Neuroendocrinology and Neuroscience from a mathematical perspective. The choice and subsequent study of appropriate mathematical formalisms to investigate these dynamics is at the core of MYCENAE's scientific foundations: slow-fast dynamical systems with multiple time scales, mean-field approaches subject to limit-size and stochastic effects, transport-like partial differential equations (PDE) and stochastic individual based models (SIBM).

The scientific positioning of MYCENAE is on the way between Mathematical Biology and Mathematics: we are involved both in the modeling of physiological processes and in the deep mathematical analysis of models, whether they be (i) models developed (or under development) within the team (ii) models developed by collaborating teams or (iii) benchmark models from the literature.

Our research program is grounded on previous results obtained in the framework of the REGATE (REgulation of the GonAdoTropE axis) Large Scale Initiative Action and the SISYPHE project team on the one hand, and the Mathematical Neuroscience Team in the Center for Interdisciplinary Research in Biology (Collège de France), on the other hand. Several of our research topics are related to the study and generalization of 2 master models: a 4D, multiscale in time, nonlinear model based on coupled FitzHugh-Nagumo dynamics that has proved to be a fruitful basis for the study of the complex oscillations in hypothalamic GnRH dynamics [34], [33], and a nD, multiscale in space, system of weakly-coupled non conservative transport equations that underlies our approach of gonadal cell dynamics [35],[7]. Most our topics in mathematical neuroscience deal with the study of complex oscillatory behaviors exhibited either by single neurons or as emergent macroscopic properties of neural networks, from both a deterministic and stochastic viewpoint.

3.2. Numerical and theoretical studies of slow-fast systems with complex oscillations

In dynamical systems with at least three state variables, the presence of different time scales favors the appearance of complex oscillatory solutions. In this context, with (at least) two slow variables MixedMode Oscillations (MMO) dynamics can arise. MMOs are small and large amplitude oscillations combined in a single time series. The last decade has witnessed a significant amount of research on this topic, including studies of folded singularities, construction of MMOs using folded singularities in combination with global dynamics, effects of additional time scales, onset of MMOs via singular Hopf bifurcations, as well as generalization to higher dimensions. In the same period, many applications to neuroscience emerged [8]. On the other hand, bursting oscillations, another prototype of complex oscillations can occur in systems with (at least) two fast variables. Bursting has been observed in many biological contexts, in particular in the dynamics of pancreatic cells, neurons, and other excitable cells. In neuronal dynamics a burst corresponds to a series of spikes, interspersed with periods of quiescent behavior, called inter-burst intervals. We are interested in systems combining bursting, MMOs and canards. One of the interesting directions is torus canards, which are canard-like structures occurring in systems combining canard explosion with fast rotation [4]. Torus canards help understand transitions from spiking or MMO dynamics to bursting. Another study on the boundary of bursting and MMOs is the work of [37] on the so-called plateau bursting. A major challenge in this direction is to gain a complete understanding of the transition from "3 time scales" to "2 fast/ 1 slow" (bursting) and then to "1 fast/ 2 slow (MMOs)". Also, a key challenge that we intend to tackle in the next few years is that of large dynamical systems with many fast and many slow variables, which additionally are changing in time and/or in phase space. We aim to pursue this research direction both at theoretical and computational level, using numerical continuation approaches based on the location of unstable trajectories by using fixed point methods, rather than simulation, to locate trajectories.

3.3. Non conservative transport equations for cell population dynamics

Models for physiologically-structured populations can be considered to derive from the so-called McKendrick-Von Foerster equation or renewal equation that has been applied and generalized in different applications of population dynamics, including ecology, epidemiology and cell biology. Renewal equations are PDE transport equations that are written so as to combine conservation laws (e.g. on the total number of individuals) with additional terms related to death or maturation, that blur the underlying overall balance law.

The development of ovarian follicles is a tightly-controlled physiological and morphogenetic process, that can be investigated from a middle-out approach starting at the cell level. To describe the terminal stages of follicular development on a cell kinetics basis and account for the selection process operated amongst follicles, we have developed a multiscale model describing the cell density in each follicle, that can be roughly considered as a system of weakly-coupled, non conservative transport equations with controlled velocities and source term. Even if, in some sense, this model belongs to the class of renewal equations for structured populations, it owns a number of specificities that render its theoretical and numerical analysis particularly challenging: 2 structuring variables (per follicle, leading as a whole to $2n$D system), control terms operating on the velocities and source term, and formulated from moments of the unknowns, discontinuities both in the velocities and density on internal boundaries of the domain representing the passage from one cell phase to another.

On the theoretical ground, the well-posedness (existence and uniqueness of weak solutions with bounded initial data) has been established in [11], while associated control problems have been studied in the framework of hybrid optimal control [5]. On the numerical ground, the formalism dedicated to the simulation of these hyperbolic-like PDEs is that of finite volume method. Part of the numerical strategy consists in combining in the most efficient way low resolution numerical schemes (such as the first-order Godunov scheme), that tend to be diffusive, with high resolution schemes (such as the Lax Wendroff second-order scheme), that may engender oscillations in the vicinity of discontinuities [2], with a critical choice of the limiter functions. The 2D finite volume schemes are combined with adaptive mesh refinement through a multi-resolution method [3] and implemented in a problem-specific way on parallel architecture [1].

3.4. Macroscopic limits of stochastic neural networks and neural fields

The coordinated activity of the cortex is the result of the interactions between a very large number of cells. Each cell is well described by a dynamical system, that receives non constant input which is the superposition of an external stimulus, noise and interactions with other cells. Most models describing the emergent behavior arising from the interaction of neurons in large-scale networks have relied on continuum limits ever since the seminal work of Wilson and Cowan and Amari [38], [32]. Such models tend to represent the activity of the network through a macroscopic variable, the population-averaged firing rate.

In order to rationally describe neural fields and more generally large cortical assemblies, one should yet base their approach on what is known of the microscopic neuronal dynamics. At this scale, the equation of the activity is a set of stochastic differential equations in interaction. Obtaining the equations of evolution of the effective mean-field from microscopic dynamics is a very complex problem which belongs to statistical physics. As in the case of the kinetic theory of gases, macroscopic states are defined by the limit of certain quantities as the network size tends to infinity. When such a limit theorem is proved, one can be ensured that large networks are well approximated by the obtained macroscopic system. Qualitative distinctions between the macroscopic limit and finite-sized networks (finite-size effects), occurs in such systems. We have been interested in the relevant mathematical approaches dealing with macroscopic limits of stochastic neuronal networks, that are expressed in the form of a complex integro-differential stochastic implicit equations of McKean-Vlasov type including a new mathematical object, the spatially chaotic Brownian motion [14].

The major question consists in establishing the fundamental laws of the collective behaviors cortical assemblies in a number of contexts motivated by neuroscience, such as communication delays between cells [13], [12] or spatially extended areas, which is the main topic of our current research. In that case additional difficulties arise, since the connection between different neurons, as well as delays in communications, depend on space in a correlated way, leading to the singular dependence of the solutions in space, which is not measurable.

NEUROSYS Project-Team

3. Research Program

3.1. Main Objectives

The main challenge in computational neuroscience is the high complexity of neural systems. The brain is a complex system and exhibits a hierarchy of interacting subunits. On a specific hierarchical level, such subunits evolve on a certain temporal and spatial scale. The interactions of small units on a low hierarchical level build up larger units on a higher hierarchical level evolving on a slower time scale and larger spatial scale. By virtue of the different dynamics on each hierarchical level, until today the corresponding mathematical models and data analysis techniques on each level are still distinct. Only few analysis and modeling frameworks are known which link successfully at least two hierarchical levels.

Once having extracted models for different description levels, typically they are applied to obtain simulated activity which is supposed to reconstruct features in experimental data. Although this approach appears straightforward, it presents various difficulties. Usually the models involve a large set of unknown parameters which determine the dynamical properties of the models. To optimally reconstruct experimental features, it is necessary to formulate an inverse problem to extract optimally such model parameters from the experimental data. Typically this is a rather difficult problem due to the low signal-to-noise ratio in experimental brain signals. Moreover, the identification of signal features to be reconstructed by the model is not obvious in most applications. Consequently an extended analysis of the experimental data is necessary to identify the interesting data features. It is important to combine such a data analysis step with the parameter extraction procedure to achieve optimal results. Such a procedure depends on the properties of the experimental data and hence has to be developed for each application separately. Machine learning approaches that attempt to mimic the brain and its cognitive processes had a lot of success in classification problems during the last decade. These hierarchical and iterative approaches use non-linear functions, which imitate neural cell responses, to communicate messages between neighboring layers. In our team, we work towards developing polysomnography-specific classifiers that might help in linking the features of particular interest for building systems for sleep signal classification with sleep mechanisms, with the accent on memory consolidation during the Rapid Eye Movement (REM) sleep phase.

3.2. Challenges

Eventually the implementation of the models and analysis techniques achieved promises to be able to construct novel data monitors. This construction involves additional challenges and stipulates the contact to realistic environments. By virtue of the specific applications of the research, the close contact to hospitals and medical enterprises shall be established in a longer term in order to (i) gain deeper insight into the specific application of the devices and (ii) build specific devices in accordance to the actual need. Collaborations with local and national hospitals and the pharmaceutical industry already exist.

3.3. Research Directions

- From the microscopic to the mesoscopic scale:
  One research direction focuses on the *relation of single neuron activity* on the microscopic scale *to the activity of neuronal populations*. To this end, the team investigates the stochastic dynamics of single neurons subject to external random inputs and involving random microscopic properties, such as random synaptic strengths and probability distributions of spatial locations of membrane ion channels. Such an approach yields a stochastic model of single neurons and allows the derivation of a stochastic neural population model.

  This bridge between the microscopic and mesoscopic scale may be performed via two pathways. The analytical and numerical treatment of the microscopic model may be called a *bottom-up approach*, since it leads to a population activity model based on microscopic activity. This approach allows theoretical neural population activity to be compared to experimentally obtained population activity. The *top-down approach* aims at extracting signal features from experimental data gained from neural populations which give insight into the dynamics of neural populations and the underlying microscopic activity. The work on both approaches represents a well-balanced investigation of the neural system based on the systems properties.

- From the mesoscopic to the macroscopic scale:
  The other research direction aims to link neural population dynamics to macroscopic activity and behaviour or, more generally, to phenomenological features. This link is more indirect but a very powerful approach to understand the brain, e.g., in the context of medical applications. Since real neural systems, such as in mammals, exhibit an interconnected network of neural populations, the team studies analytically and numerically the network dynamics of neural populations to gain deeper insight into possible phenomena, such as traveling waves or enhancement and diminution of certain neural rhythms. Electroencephalography (EEG) is a wonderful brain imaging technique to study the overall brain activity in real time non-invasively. However it is necessary to develop robust techniques based on stable features by investigating the time and frequency domains of brain signals. Two types of information are typically used in EEG signals: (i) transient events such as evoked potentials, spindles and K-complexes and (ii) the power in specific frequency bands.

NUMED Project-Team

3. Research Program

3.1. Multiscale propagation phenomena in biology

3.1.1. Project team positioning

The originality of our work is the quantitative description of propagation phenomena accounting for several time and spatial scales. Here, propagation has to be understood in a broad sense. This includes propagation of invasive species, chemotactic waves of bacteira, evoluation of age structures populations ... Our main objectives are the quantitative calculation of macroscopic quantities as the rate of propagation, and microscopic distributions at the edge and the back of the front. These are essential features of propagation which are intimately linked in the long time dynamics.

Multiscale modeling of propagation phenomena raises a lot of interest in several fields of application. This ranges from shock waves in kinetic equations (Boltzmann, BGK, etc...), bacterial chemotactic waves, selection-mutation models with spatial heterogeneities, evolution in age-structured population or subdiffusive processes.

Earlier works generally focused on numerical simulations, hydrodynamic limits to average over the microscopic variable, or specific models with only local features, not suitable for most of the relevant biological situations. Our contribution enables to derive the relevant features of propagation analytically, and far from the hydrodynamic regime for a wide range of models including nonlocal interaction terms.

Our recent understanding is closely related to the analysis of large deviations in multiscale dispersion equations (e.g. PDMP), for which we gave important contributions too in collaboration with E. Bouin (CEREMADE Dauphine), E. Grenier (Inria NUMED) and G. Nadin (Univ. Paris 6).

These advances are linked to the work of other Inria teams (MAMBA, DRACULA, BEAGLE), and collaborators in mathematics, physics and theoretical biology in France, Austria and UK.

3.1.2. Recent results

Vincent Calvez has focused on the modelling and analysis of propagation phenomena in structured populations. This includes chemotactic concentration waves, transport-reaction equations, coupling between ecological processes (reaction-diffusion) and evolutionary processes (selection of the fittest trait, adaptation), evolution of age structured poulations, and anomalous diffusion. As a main result, he could establish the existence of concentration waves of chemotactic bacteria E. coli in a fully coupled kinetic/reaction-diffusion system previously validated on experimental data.

In collaboration with a group of theoretical biologists at ISEM Montpellier (O. Ronce and O. Cotto), and J. Garnier (Univ. Savoie), Th. Lepoutre (Inria DRACULA), Th. Bourgeron (Inria NUMED) he has investigated quantitatively the maladaptation of an age-structured population in a changing environment. He has unravelled a striking phenomenon of severe maladaptation specific to age structure. This was observed on numerical simulations by biologists, but it has now a systematic mathematical comprehension.

He has also continued his work on the optimal control of monotone linear dynamical systems, using the Hamilton-Jacobi framework, and the weak KAM theory, in collaboration with P. Gabriel (UVSQ) and S. Gaubert (Inria MAXPLUS).

Alvaro Mateos Gonzalez has started his PhD on September 2014 under the supervision of Vincent Calvez, and Hugues Berry (BEAGLE), . He has already collaborated fruitfully with Thomas Lepoutre (DRACULA) and Hugues Berry to investigate the long-time asymptotics of a degenerate renewal equation. This is a first step towards the mathematical analysis of anomalous diffusion processes. In collaboration with P. Gabriel (UVSQ) and V. Calvez (Inria NUMED) he has investigated large deviations of heterogenous continuous time random walks.

3.1.3. Collaborations

- Mathematical description of bacterial chemotactic waves:
  - **N. Bournaveas** (Univ. Edinburgh), **V. Calvez** (ENS de Lyon, Inria NUMED) **B. Perthame** (Univ. Paris 6, Inria BANG), **Ch. Schmeiser** (Univ. Vienna), **N. Vauchelet**: design of the model, analysis of traveling waves, analysis of optimal strategies for bacterial foraging.
  - **J. Saragosti**, **V. Calvez** (ENS de Lyon, Inria NUMED), **A. Buguin**, **P. Silberzan** (Institut Curie, Paris): experiments, design of the model, identification of parameters.
- Transport-reaction waves and large deviations:
  - **E. Bouin**, **V. Calvez** (ENS de Lyon, Inria NUMED), **E. Grenier** (ENS de Lyon, Inria NUMED), **G. Nadin** (Univ. Paris 6)
- Selection-mutation models of invasive species:
  - **E. Bouin** (ENS de Lyon, Inria NUMED), **V. Calvez** (ENS de Lyon, Inria NUMED), **S. Mirrahimi** (Inst. Math. Toulouse): construction of traveling waves, asymptotic propagation of fronts,
  - **E. Bouin** (ENS de Lyon, Inria NUMED), **V. Calvez** (ENS de Lyon, Inria NUMED), **N. Meunier**, (Univ. Paris 5), **B. Perthame** (Univ. Paris 6, Inria Bang), **G. Raoul** (CEFE, Montpellier), **R. Voituriez** (Univ. Paris 6): formal analysis, derivation of various asymptotic regimes.
- Age-structured equations for anomalous diffusion processes, and evolution
  - **H. Berry** (Inria BEAGLE), **V. Calvez** (ENS de Lyon, Inria NUMED), **Th. Lepoutre** (Inria DRACULA), **P. Gabriel** (Univ. UVSQ), O. Ronce (ISEM Montpellier), O. Cotto (ISEM Montpellier), J. Garnier (Univ. Savoie).

3.2. Growth of biological tissues

3.2.1. Project-team positioning

The originality of our work is the derivation, analysis and numerical simulations of mathematical model for growing cells and tissues. This includes mechanical effects (growth induces a modification of the mechanical stresses) and biological effects (growth is potentially influenced by the mechanical forces).

This leads to innovative models, adapted to specific biological problems (*e.g.* suture formation, cell polarisation), but which share similar features. We perform linear stability analysis, and look for pattern formation issues (at least instability of the homogeneous state).

The biophysical literature of such models is large. We refer to the groups of Ben Amar (ENS Paris), Boudaoud (ENS de Lyon), Mahadevan (Harvard), etc.

Our team combines strong expertise in reaction-diffusion equations (V. Calvez) and mechanical models (P. Vigneaux). We develop linear stability analysis on evolving domains (due to growth) for coupled biomechanical systems.

Another direction of work is the mathematical analysis of classical tumor growth models. These continuous mechanics models are very close to classical equations like Euler or Navier Stokes equations in fluid mechanics. However they bring there own difficulties: Darcy law, multispecies equations, non newtonian dynamics (Bingham flows). Part of our work consist in deriving existence results and designing acute numerical schemes for these equations.

3.2.2. Recent results

We have worked on several biological issues. Cell polarisation is the main one. We first analyzed a nonlinear model proposed by theoretical physicists and biologists to describe spontaneous polarisation of the budding yeast *S. cerevisae*. The model assumes a dynamical transport of molecules in the cytoplasm. It is analogous to the Keller-Segel model for cell chemotaxis, except for the source of the transport flux. We developped nonlinear analysis and entropy methods to investigate pattern formation (Calvez et al 2012). We are currently validating the model on experimental data. The analysis of polarization of a single cell is a preliminary step before the study of mating in a population of yeast cells. In the mating phase, secretion of pheromones induces a dialogue between cells of opposite types.

We also derive realistic models for the growth of the fission yeast *S. pombe*. We proposed two models which couple growth and geometry of the cell. We aim to tackle the issue of pattern formation, and more specifically the instability of the spherical shape, leading to a rod shape. The mechanical coupling involves the distribution of microtubules in the cytoplasm, which bring material to the cell wall.

Over the evaluation period, Paul Vigneaux developped expertise in modelling and design of new numerical schemes for complex fluid models of the viscoplastic type. Associated materials are involved in a broad range of applications ranging from chemical industry to geophysical and biological materials. In the context of NUMED, this expertise is linked to the development of complex constitutive laws for cancer cell tissue. During the period, NUMED used mixed compressible/incompressible fluid model for tumor growth and viscoelastic fluid model. Viscoplastic is one of the other types of complex fluid model which is usable in the field. Mathematically, it involves variational inequalities and the need for specific numerical methods.

3.2.3. Collaborations

- **V. Calvez** (ENS de Lyon, Inria NUMED), **Th. Lepoutre** (Inria DRACULA), **N. Meunier**, (Univ. Paris 5), **N. Muller** (Univ. Paris 5), **P. Vigneaux** (ENS de Lyon, Inria NUMED): mathematical analysis of cell polarisation, numerical simulations
- **V. Calvez** (ENS de Lyon, Inria NUMED), **N. Meunier**, (Univ. Paris 5), **M. Piel**, (Institut Curie, Paris), **R. Voituriez** (Univ. Paris 6): biomechanical modeling of the growth of *S. pombe*
- **D. Bresch** (Univ. Chambéry), **V. Calvez** (ENS de Lyon, Inria NUMED), **R.H. Khonsari** (King's College London, CHU Nantes), **J. Olivier** (Univ. Aix-Marseille), **P. Vigneaux** (ENS de Lyon, Inria NUMED): modeling, analysis and simulations of suture formation.
- **Didier Bresch** (Univ Chambéry), **Benoit Desjardins**(Moma group): petrology.

ANR JCJC project "MODPOL", *Mathematical models for cell polarization*, led by Vincent Calvez (ENS de Lyon, CNRS, Inria NUMED).

3.3. Multiscale models in oncology

3.3.1. Project-team positioning

Since 15 years, the development of mathematical models in oncology has become a significant field of research throughout the world. Several groups of researchers in biomathematics have developed complex and multiscale continuous and discrete models to describe the pathological processes as well as the action of anticancer anticancer drugs. Many groups in US (e.g. Alexander Anderson's lab, Kristin Swansson's lab) and in Canada (e.g. Thomas Hillen, Gerda de Vries), quickly developed and published interesting modeling frameworks. The setup of European networks such as the Marie Curie research and training networks managed by Nicolas Bellomo and Luigi Preziosi constituted a solid and fertile ground for the development of new oncology models by teams of biomathematicians and in particular Zvia Agur (Israel), Philip Maini (UK), Helen Byrne (UK), Andreas Deutsch (Germany), or Miguel Herrero (Spain).

3.3.2. Results

We have worked on the development of a multiscale system for modeling the complexity of the cancer disease and generate new hypothesis on the use of anti-cancer drugs. This model relies on a multiscale formalism integrating a subcellular level integrating molecular interactions, a cell level (integrating the regulation of the cell cycle at the levels of individual cells) and a macroscopic level for describing the spatio-temporal dynamics of different types of tumor tissues (proliferating, hypoxic and necrotic). The model is thus composed by a set of partial differential equations (PDEs) integrating molecular network up to tissue dynamics using lax from fluid dynamic. This formalism is useful to investigate theoretically different cancer processes such as the angiogenesis and invasion. We have published several examples and case studies of the use of this model in particular, the action of phase-specific chemotherapies (Ribba, You et al. 2009), the use of anti-angiogenic drugs (Billy, Ribba et al. 2009) and their use in combination with chemotherapies (Lignet, Benzekry et al. 2013). This last work also integrates a model of the VEGF molecular pathway for proliferation and migration of endothelial cells in the context of cancer angiogenesis (Lignet, Calvez et al. 2013).

If these types of models present interesting framework to theoretically investigate biological hypothesis, they however present limitation due to their large number of parameters. In consequence, we decided to stop the development of the multiscale platform until exploration of alternative modeling strategies to deal with real data. We focus our interest on the use of mixed-effect modeling techniques as classically used in the field of pharmacokinetic and pharmacodynamics modeling. The general principal of this approach lies in the integration of several levels of variability in the model thus allowing for the simultaneous analysis of data in several individuals. Nowadays, complex algorithms allow for dealing with this problem when the model is composed by few ordinary differential equations (ODEs). However, no similar parameter estimation method is available for models defined as PDEs. In consequence, we decided: 1. To develop more simple models, based on systems of ODEs, assuming simplistic hypothesis of tumor growth and response to treatment but with a real focus on model ability to predict real data. 2. To work alone the development of parameter estimation methods for PDE models in oncology.

3.4. Parametrization of complex systems

3.4.1. Project-team positioning

We focus on a specific problem: the "population" parametrization of a complex system. More precisely, instead of trying to look for parameters in order to fit the available data for one patient, in many cases it is more pertinent to look for the distribution of the parameters (assuming that it is gaussian or log gaussian) in a population of patients, and to maximize the likelihood of the observations of all patients. It is a very useful strategy when few data per patients are available, but when we have a lot of patients. The number of parameters to find is multiplied by two (average and standard deviation for each parameter) but the number of data is greatly increased.

This strategy, that we will call "population" parametrization has been initiated in the eighties by software like Nonmem. Recently Marc Lavielle (Popix team) made a series of breakthroughs and designed a new powerfull algorithm, leading to Monolix software.

However population parametrization is very costly. It requires several hundred of thousands of model evaluations, which may be very long.

3.4.2. Results

We address the problem of computation time when the complex model is long to evaluate. In simple cases like reaction diffusion equations in one space dimension, the evaluation of the model may take a few seconds of even a few minutes. In more realistic geometries, the computation time would be even larger and can reach the hour or day. It is therefore impossible to run a SAEM algorith on such models, since it would be much too long. Moreover the underlying algorithm can not be parallelized.

We propose a new iterative approach combining a SAEM algorithm together with a kriging. This strategy appears to be very efficient, since we were able to parametrize a PDE model as fast as a simple ODE model.

We are currently developing the corresponding software.

3.5. Models for the analysis of efficacy data in oncology

3.5.1. Project-team positioning

The development of new drugs for oncology patients faces significant issues with a global attrition rate of 95 percents and only 40 percents of drug approval in phase III after successful phase II. As for meteorology, the analysis through modeling and simulation (MS), of time-course data related to anticancer drugs efficacy and/or toxicity constitutes a rational method for predicting drugs efficacy in patients. This approach, now supported by regulatory agencies such as the FDA, is expected to improve the drug development process and in consequence the treatment of cancer patients. A private company, Pharsight, has nowadays the leader team in the development of such modeling frameworks. In 2009, this team published a model describing tumor size time-course in more than one thousand colorectal cancer patients. This model was used in an MS framework to predict the outcome of a phase III clinical trials based on the analysis of phase II data. From 2009 to 2013, 12 published articles address similar analysis of different therapeutic indications such as lung, prostate, thyroid and renal cancer. A similar modeling activity is also proposed for the analysis of data in preclinical experiments, and in particular, experiments in mice. Animal experiments represent critical stages to decide if a drug molecule should be tested in humans. MS methods are considered as tools to better investigate the mechanisms of drug action and to potentially facilitate the transition towards the clinical phases of the drug development process. Our team has worked in the development of two modeling frameworks with application in both preclinical and clinical oncology. For the preclinical context, we have worked on the development of models focusing on the process of tumor angiogenesis, i.e. the formation of intra-tumoral blood vessels. At the clinical level, we have developed a model to predict tumor size dynamics in patients with low-grade glioma.

At Inria, several project-teams have developed similar efforts. The project-team BANG has a solid experience in the development of age-structured models of the cell cycle and tissue regulation of tumors with clinical applications for chronotherapy. BANG is also currently applying these types of partial differential equation (PDE) models to the study of leukemia through collaboration with the project-team DRACULA. Project-team MC2 has recently shown that the analysis, through a simplified PDE model of tumor growth and treatment response, of 3D imaging, could lead to correct prediction of tumor volume evolution in patients with pulmonary metastasis from thyroid cancer. Regarding specifically the modeling of brain tumors, project-team ASCLEPIOS has brought an important contribution towards personalized medicine in analyzing 3D data information from MRI with a multiscale model that describes the evolution of high grade gliomas in the brain. Their framework relies on the cancer physiopathological model that was mainly developed by Kristin Swanson and her group at the university of Washington.

Outside from Inria, we wish to mention here the work of the group of Florence Hubert in Marseille in the development of models with an interesting compromise between mathematical complexity and data availability. A national ANR project led by the team is expected to support the development of an MS methodology for the analysis of tumor size data in patients with metastases.

3.5.2. Results

Regarding our contribution in preclinical modeling, we have developed a model to analyze the dynamics of tumor progression in nude mice xenografted with HT29 or HCT116 colorectal cancer cells. This model, based on a system of ordinary differential equations (ODEs), integrated the different types of tumor tissues, and in particular, the proliferating, hypoxic and necrotic tissues. Practically, in our experiment, tumor size was periodically measured, and percentages of hypoxic and necrotic tissue were assessed using immunohistochemistry techniques on tumor samples after euthanasia. In the proposed model, the peripheral non-hypoxic tissue proliferates according to a generalized-logistic equation where the maximal tumor size is represented by a variable called "carrying capacity". The ratio of the whole tumor size to the carrying capacity was used to define the hypoxic stress. As this stress increases, non-hypoxic tissue turns hypoxic. Hypoxic tissue does not stop proliferating, but hypoxia constitutes a transient stage before the tissue becomes necrotic. As the tumor grows, the carrying capacity increases owing to the process of angiogenesis (Ribba, Watkin et al. 2011). The model is shown to correctly predict tumor growth dynamics as well as percentages of necrotic and hypoxic tissues within the tumor.

Regarding our contribution in clinical oncology, we developed an ODE model based on the analysis of mean tumor diameter (MTD) time-course in low-grade glioma patients (Ribba, Kaloshi et al. 2012).

In this model, the tumor is composed of proliferative (P) and non-proliferative quiescent tissue (Q) expressed in millimeters. The proportion of proliferative tissue transitioning into quiescence is constant. The treatment directly eliminates proliferative cells by inducing lethal DNA damage while these cells progress through the cell cycle. The quiescent cells are also affected by the treatment and become damaged quiescent cells (k_{PQ}). Damaged quiescent cells, when re-entering the cell cycle, can repair their DNA and become proliferative once again (transition from Q_P to P) or can die due to unrepaired damages. We modeled the pharmacokinetics of the PCV chemotherapy using a kinetic-pharmacodynamic (K-PD) approach, in which drug concentration is assumed to decay according to an exponential function. In this model, we did not consider the three drugs separately. Rather, we assumed the treatment to be represented as a whole by a unique variable (C), which represents the concentration of a virtual drug encompassing the three chemotherapeutic components of the PCV regimen. We modeled the exact number of treatment cycles administered by setting the value of C to 1 (arbitrary unit) at the initiation of each cycle(T_{Treat}): $C(T = T_{Treat}) = 1$.

The resulting model is as follows:

$$\begin{aligned} \frac{dC}{dt} &= -KDE \times C \\ \frac{dP}{dt} &= \lambda_P P \left(1 - \frac{P^{\star}}{K}\right) + k_{Q_pP} Q_p - k_{PQ} P - \gamma \times C \times KDE \times P \\ \frac{dQ}{dt} &= k_{PQ} P - \gamma \times C \times KDE \times Q \\ \frac{dQ_p}{dt} &= \gamma \times C \times KDE \times Q - k_{Q_pP} Q_p - \delta_{Q_p} Q_p \end{aligned} \tag{82}$$

We challenged this model with additional patient data. In particular, MTD time-course information from 24 patients treated with TMZ (subset of the 120 patients from SH) and 25 patients treated with radiotherapy (SH). Note that exactly the same K-PD approach was used to model treatment pharmacokinetic (including for radiotherapy). This choice, though not really realistic was adopted for simplicity reasons: the same model can be indifferently applied to the three different treatment modalities of LGG patients.

3.5.3. Collaborations

François Ducray and Jérôme Honnorat (Pierre Wertheimer Hospital in Lyon)

External support: grant INSERM PhysiCancer 2012 and Inria IPL MONICA

3.6. Stroke

3.6.1. Project team positioning

Stroke is a major public health problem since it represents the second leading cause of death worldwide and the first cause of acquired disability in adults.

Numed is currently starting completely new issues with D. Rousseau (INSA) and his team. We have now at hand a large data base of clinical images. Our aim is to develop model which are able to predict the final size of the dead brain area as a function of the first two clinical data.

PARIETAL Project-Team

3. Research Program

3.1. Inverse problems in Neuroimaging

Many problems in neuroimaging can be framed as forward and inverse problems. For instance, brain population imaging is concerned with the *inverse problem* that consists in predicting individual information (behavior, phenotype) from neuroimaging data, while the corresponding *forward problem* boils down to explaining neuroimaging data with the behavioral variables. Solving these problems entails the definition of two terms: a loss that quantifies the goodness of fit of the solution (does the model explain the data well enough ?), and a regularization scheme that represents a prior on the expected solution of the problem. These priors can be used to enforce some properties on the solutions, such as sparsity, smoothness or being piece-wise constant.

Let us detail the model used in typical inverse problem: Let $\mathbf{X}$ be a neuroimaging dataset as an $(n_{subjects}, n_{voxels})$ matrix, where $n_{subjects}$ and n_{voxels} are the number of subjects under study, and the image size respectively, $\mathbf{Y}$ a set of values that represent characteristics of interest in the observed population, written as $(n_{subjects}, n_{features})$ matrix, where $n_{features}$ is the number of characteristics that are tested, and β an array of shape $(n_{voxels}, n_{features})$ that represents a set of pattern-specific maps. In the first place, we may consider the columns $\mathbf{Y}_1, .., \mathbf{Y}_{n_{features}}$ of Y independently, yielding $n_{features}$ problems to be solved in parallel:

$$\mathbf{Y}_i = \mathbf{X}\beta_i + \epsilon_i, \forall i \in \{1, .., n_{features}\},$$

where the vector contains β_i is the i^{th} row of β. As the problem is clearly ill-posed, it is naturally handled in a regularized regression framework:

$$\widehat{\beta}_i = \text{argmin}_{\beta_i} \|\mathbf{Y}_i - \mathbf{X}\beta_i\|^2 + \Psi(\beta_i), \tag{83}$$

where Ψ is an adequate penalization used to regularize the solution:

$$\Psi(\beta; \lambda_1, \lambda_2, \eta_1, \eta_2) = \lambda_1\|\beta\|_1 + \lambda_2\|\beta\|_2 + \eta_1\|\nabla\beta\|_{2,1} + \eta_2\|\nabla\beta\|_{2,2} \tag{84}$$

with λ_1, λ_2, η_1, $\eta_2 \geq 0$ (this formulation particularly highlights the fact that convex regularizers are norms or quasi-norms). In general, only one or two of these constraints is considered (hence is enforced with a non-zero coefficient):

- When $\lambda_1 > 0$ only (LASSO), and to some extent, when $\lambda_1, \lambda_2 > 0$ only (elastic net), the optimal solution β is (possibly very) sparse, but may not exhibit a proper image structure; it does not fit well with the intuitive concept of a brain map.
- Total Variation regularization (see Fig. 1) is obtained for ($\eta_1 > 0$ only), and typically yields a piece-wise constant solution. It can be associated with Lasso to enforce both sparsity and sparse variations.
- Smooth lasso is obtained with ($\eta_2 > 0$ and $\lambda_1 > 0$ only), and yields smooth, compactly supported spatial basis functions.

Note that, while the qualitative aspect of the solutions are very different, the predictive power of these models is often very close.

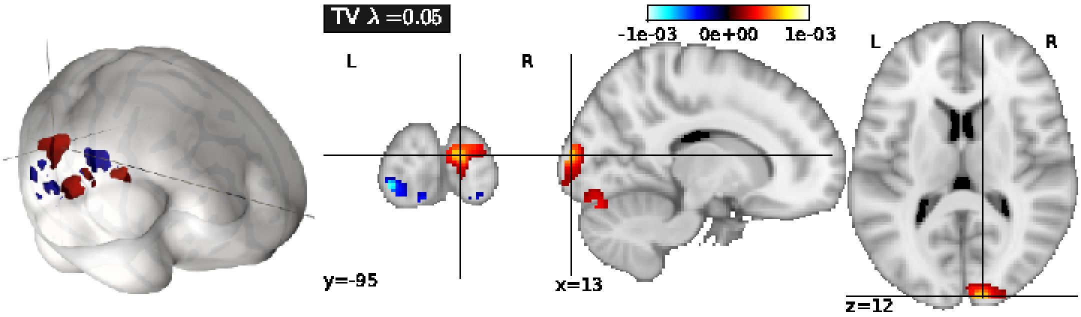

Figure 1. Example of the regularization of a brain map with total variation in an inverse problem. The problem here is to predict the spatial scale of an object presented as a stimulus, given functional neuroimaging data acquired during the presentation of an image. Learning and test are performed across individuals. Unlike other approaches, Total Variation regularization yields a sparse and well-localized solution that also enjoys high predictive accuracy.

The performance of the predictive model can simply be evaluated as the amount of variance in $\mathbf{Y}_i$ fitted by the model, for each $i \in \{1,..,n_{features}\}$. This can be computed through cross-validation, by *learning*$\widehat{\beta}_i$ on some part of the dataset, and then estimating $\|\mathbf{Y}_i - \mathbf{X}\widehat{\beta}_i\|^2$ using the remainder of the dataset.

This framework is easily extended by considering

- *Grouped penalization*, where the penalization explicitly includes a prior clustering of the features, i.e. voxel-related signals, into given groups. This amounts to enforcing structured priors on the problem solution.
- *Combined penalizations*, i.e. a mixture of simple and group-wise penalizations, that allow some variability to fit the data in different populations of subjects, while keeping some common constraints.
- *Logistic and hinge regression*, where a non-linearity is applied to the linear model so that it yields a probability of classification in a binary classification problem.
- *Robustness to between-subject variability* to avoid the learned model overly reflecting a few outlying particular observations of the training set. Note that noise and deviating assumptions can be present in both $\mathbf{Y}$ and $\mathbf{X}$
- *Multi-task learning*: if several target variables are thought to be related, it might be useful to constrain the estimated parameter vector β to have a shared support across all these variables.
  For instance, when one of the variables $\mathbf{Y}_i$ is not well fitted by the model, the estimation of other variables $\mathbf{Y}_j, j \neq i$ may provide constraints on the support of β_i and thus, improve the prediction of $\mathbf{Y}_i$.

$$\mathbf{Y} = \mathbf{X}\beta + \epsilon, \tag{85}$$

then

$$\widehat{\beta} = \text{argmin}_{\beta=(\beta_i),i=1..n_f} \sum_{i=1}^{n_f} \|\mathbf{Y_i} - \mathbf{X}\beta_\mathbf{i}\|^2 + \lambda \sum_{j=1}^{n_{voxels}} \sqrt{\sum_{i=1}^{n_f} \beta_{\mathbf{i,j}}^{\mathbf{2}}} \tag{86}$$

3.2. Multivariate decompositions

Multivariate decompositions provide a way to model complex data such as brain activation images: for instance, one might be interested in extracting an *atlas of brain regions* from a given dataset, such as regions exhibiting similar activity during a protocol, across multiple protocols, or even in the absence of protocol (during resting-state). These data can often be factorized into spatial-temporal components, and thus can be estimated through *regularized Principal Components Analysis* (PCA) algorithms, which share some common steps with regularized regression.
Let $\mathbf{X}$ be a neuroimaging dataset written as an $(n_{subjects}, n_{voxels})$ matrix, after proper centering; the model reads

$$\mathbf{X} = \mathbf{AD} + \epsilon, \tag{87}$$

where $\mathbf{D}$ represents a set of n_{comp} spatial maps, hence a matrix of shape (n_{comp}, n_{voxels}), and $\mathbf{A}$ the associated subject-wise loadings. While traditional PCA and independent components analysis are limited to reconstructing components $\mathbf{D}$ within the space spanned by the column of $\mathbf{X}$, it seems desirable to add some constraints on the rows of $\mathbf{D}$, that represent spatial maps, such as sparsity, and/or smoothness, as it makes the interpretation of these maps clearer in the context of neuroimaging. This yields the following estimation problem:

$$\text{min}_{\mathbf{D},\mathbf{A}} \|\mathbf{X} - \mathbf{AD}\|^2 + \Psi(\mathbf{D}) \text{ s.t. } \|\mathbf{A}_i\| = 1 \; \forall i \in \{1..n_{features}\}, \tag{88}$$

where $(\mathbf{A}_i)$, $i \in \{1..n_{features}\}$ represents the columns of $\mathbf{A}$. Ψ can be chosen such as in Eq. (2) in order to enforce smoothness and/or sparsity constraints.
The problem is not jointly convex in all the variables but each penalization given in Eq (2) yields a convex problem on $\mathbf{D}$ for $\mathbf{A}$ fixed, and conversely. This readily suggests an alternate optimization scheme, where $\mathbf{D}$ and $\mathbf{A}$ are estimated in turn, until convergence to a local optimum of the criterion. As in PCA, the extracted components can be ranked according to the amount of fitted variance. Importantly, also, estimated PCA models can be interpreted as a probabilistic model of the data, assuming a high-dimensional Gaussian distribution (probabilistic PCA).

Utlimately, the main limitations to these algorithms is the cost due to the memory requirements: holding datasets with large dimension and large number of samples (as in recent neuroimaging cohorts) leads to inefficient computation. To solve this issue, online method are particularly attractive.

3.3. Covariance estimation

Another important estimation problem stems from the general issue of learning the relationship between sets of variables, in particular their covariance. Covariance learning is essential to model the dependence of these variables when they are used in a multivariate model, for instance to study potential interactions between variables. Covariance learning is necessary to model latent interactions in high-dimensional observation spaces, e.g. when considering multiple contrasts or functional connectivity data.
The difficulties are two-fold: on the one hand, there is a shortage of data to learn a good covariance model from an individual subject, and on the other hand, subject-to-subject variability poses a serious challenge to the use of multi-subject data. While the covariance structure may vary from population to population, or depending on the input data (activation versus spontaneous activity), assuming some shared structure across problems, such as their sparsity pattern, is important in order to obtain correct estimates from noisy data. Some of the most important models are:

- **Sparse Gaussian graphical models**, as they express meaningful conditional independence relationships between regions, and do improve conditioning/avoid overfit.

- **Decomposable models**, as they enjoy good computational properties and enable intuitive interpretations of the network structure. Whether they can faithfully or not represent brain networks is still an open question.
- **PCA-based regularization of covariance** which is powerful when modes of variation are more important than conditional independence relationships.

Adequate model selection procedures are necessary to achieve the right level of sparsity or regularization in covariance estimation; the natural evaluation metric here is the out-of-samples likelihood of the associated Gaussian model. Another essential remaining issue is to develop an adequate statistical framework to test differences between covariance models in different populations. To do so, we consider different means of parametrizing covariance distributions and how these parametrizations impact the test of statistical differences across individuals.

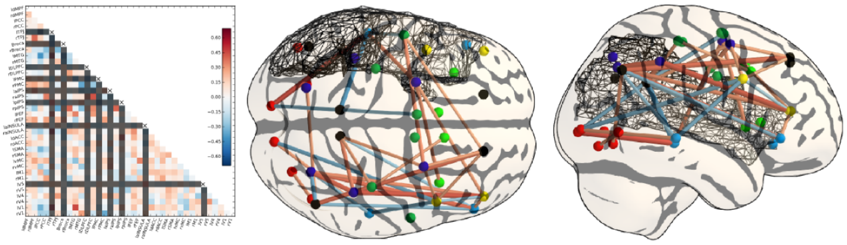

Figure 2. Example of functional connectivity analysis: The correlation matrix describing brain functional connectivity in a post-stroke patient (lesion volume outlined as a mesh) is compared to a group of control subjects. Some edges of the graphical model show a significant difference, but the statistical detection of the difference requires a sophisticated statistical framework for the comparison of graphical models.

PLEIADE Team

3. Research Program

3.1. Distances and pattern recognition

Diversity may be understood as a set of dissimilarities between objects. The underlying mathematical construction is the notion of distance. Knowing a set of objects, on the condition that pairwise distances can be measured, it is possible to build a Euclidan image of it as a point cloud in a space of relevant dimension. Then, diversity can be associated with the shape of the point cloud. It is still true that the reference for recognizing patterns or shapes is the human eye. One objective of our project is to narrow the gap between the story that a human eye can read, and the story that an algorithm can tell. Several directions will be explored. First, it is necessary to master dimension reduction, mainly classical algebraic tools (PCA, NGS, Isomap, eigenmaps, etc ...), and collaborate with experts in efficient methods in spectral methods. Second, a neighborhood in a point cloud naturally leads to graphs describing the neighborhood networks. There is a natural link between modular structures in distance arrays and communities on graphs. Third, points defined by DNA sequences (for example) are samples of diversity. Dimension reduction may show that they live on a given manifold. This leads to geometry (differential or Riemanian geometry). Knowing some properties of the manifold can inform us about the constraints on the space where the measured individuals live. The connection between Riemannian geometry and graphs, where weighted graphs are seen as meshes embedded in a manifold, is currently an active field of reasearch [33], [32].

To resolve these objectives computationally will require investment in research directions in computational geometry (such as convex hulls of high-dimension sets of points), on circumventing the curse of dimensionality, and on linking distance geometry with convex optimization procedures through matrix completion. None of these questions is trivial: most recent work has focused on two or three dimensions, for example for image analysis or for reconstruction of protein conformation from local distances between atoms. The methodological goal is to extend these approaches to higher dimension spaces.

3.2. Modeling by successive refinement

Describing the links between diversity in traits and diversity in function will require comprehensive models, assembled from and refining existing models. A recurring difficulty in building comprehensive models of biological systems is that accurate models for subsystems are built using different formalisms and simulation techniques, and hand-tuned models tend to be so focused in scope that it is difficult to repurpose them [17]. Our belief is that a sustainable effort in building efficient behavioral models must proceed incrementally, rather than by modeling individual processes *de novo*. *Hierarchical modeling* [14] is one way of combining specific models into networks. Effective use of hierarchical models requires both formal definition of the semantics of such composition, and efficient simulation tools for exploring the large space of complex behaviors. We have previously shown that this approach can be effective for certains kinds of systems in biotechnology [2], [18] and medicine [16]. Our challenge is to adapt incremental, hierarchical refinement to modeling organisms and communities in metagenomic and comparative genomic applications.

REO Project-Team

3. Research Program

3.1. Multiphysics modeling

In large vessels and in large bronchi, blood and air flows are generally supposed to be governed by the incompressible Navier-Stokes equations. Indeed in large arteries, blood can be supposed to be Newtonian, and at rest air can be modeled as an incompressible fluid. The cornerstone of the simulations is therefore a Navier-Stokes solver. But other physical features have also to be taken into account in simulations of biological flows, in particular fluid-structure interaction in large vessels and transport of sprays, particles or chemical species.

3.1.1. Fluid-structure interaction

Fluid-structure coupling occurs both in the respiratory and in the circulatory systems. We focus mainly on blood flows since our work is more advanced in this field. But the methods developed for blood flows could be also applied to the respiratory system.

Here “fluid-structure interaction” means a coupling between the 3D Navier-Stokes equations and a 3D (possibly thin) structure in large displacements.

The numerical simulations of the interaction between the artery wall and the blood flows raise many issues: (1) the displacement of the wall cannot be supposed to be infinitesimal, geometrical nonlinearities are therefore present in the structure and the fluid problem have to be solved on a moving domain (2) the densities of the artery walls and the blood being close, the coupling is strong and has to be tackled very carefully to avoid numerical instabilities, (3) “naive” boundary conditions on the artificial boundaries induce spurious reflection phenomena.

Simulation of valves, either at the outflow of the cardiac chambers or in veins, is another example of difficult fluid-structure problems arising in blood flows. In addition, very large displacements and changes of topology (contact problems) have to be handled in those cases.

Due to stability reasons, it seems impossible to successfully apply in hemodynamics the explicit coupling schemes used in other fluid-structure problems, like aeroelasticity. As a result, fluid-structure interaction in biological flows raise new challenging issues in scientific computing and numerical analysis : new schemes have to be developed and analyzed.

We have proposed and analyzed over the last few years several efficient fluid-structure interaction algorithms. This topic remains very active. We are now using these algorithms to address inverse problems in blood flows to make patient specific simulations (for example, estimation of artery wall stiffness from medical imaging).

3.1.2. Aerosol

Complex two-phase fluids can be modeled in many different ways. Eulerian models describe both phases by physical quantities such as the density, velocity or energy of each phase. In the mixed fluid-kinetic models, the biphasic fluid has one dispersed phase, which is constituted by a spray of droplets, with a possibly variable size, and a continuous classical fluid.

This type of model was first introduced by Williams [64] in the frame of combustion. It was later used to develop the Kiva code [54] at the Los Alamos National Laboratory, or the Hesione code [59], for example. It has a wide range of applications, besides the nuclear setting: diesel engines, rocket engines [57], therapeutic sprays, *etc.* One of the interests of such a model is that various phenomena on the droplets can be taken into account with an accurate precision: collision, breakups, coagulation, vaporization, chemical reactions, *etc.*, at the level of the droplets.

The model usually consists in coupling a kinetic equation, that describes the spray through a probability density function, and classical fluid equations (typically Navier-Stokes). The numerical solution of this system relies on the coupling of a method for the fluid equations (for instance, a finite volume method) with a method fitted to the spray (particle method, Monte Carlo).

We are mainly interested in modeling therapeutic sprays either for local or general treatments. The study of the underlying kinetic equations should lead us to a global model of the ambient fluid and the droplets, with some mathematical significance. Well-chosen numerical methods can give some tracks on the solutions behavior and help to fit the physical parameters which appear in the models.

3.2. Multiscale modeling

Multiscale modeling is a necessary step for blood and respiratory flows. In this section, we focus on blood flows. Nevertheless, similar investigations are currently carried out on respiratory flows.

3.2.1. Arterial tree modeling

Problems arising in the numerical modeling of the human cardiovascular system often require an accurate description of the flow in a specific sensible subregion (carotid bifurcation, stented artery, *etc.*). The description of such local phenomena is better addressed by means of three-dimensional (3D) simulations, based on the numerical approximation of the incompressible Navier-Stokes equations, possibly accounting for compliant (moving) boundaries. These simulations require the specification of boundary data on artificial boundaries that have to be introduced to delimit the vascular district under study. The definition of such boundary conditions is critical and, in fact, influenced by the global systemic dynamics. Whenever the boundary data is not available from accurate measurements, a proper boundary condition requires a mathematical description of the action of the reminder of the circulatory system on the local district. From the computational point of view, it is not affordable to describe the whole circulatory system keeping the same level of detail. Therefore, this mathematical description relies on simpler models, leading to the concept of *geometrical multiscale* modeling of the circulation [60]. The underlying idea consists in coupling different models (3D, 1D or 0D) with a decreasing level of accuracy, which is compensated by their decreasing level of computational complexity.

The research on this topic aims at providing a correct methodology and a mathematical and numerical framework for the simulation of blood flow in the whole cardiovascular system by means of a geometric multiscale approach. In particular, one of the main issues will be the definition of stable coupling strategies between 3D and reduced order models.

To model the arterial tree, a standard way consists of imposing a pressure or a flow rate at the inlet of the aorta, *i.e.* at the network entry. This strategy does not allow to describe important features as the overload in the heart caused by backward traveling waves. Indeed imposing a boundary condition at the beginning of the aorta artificially disturbs physiological pressure waves going from the arterial tree to the heart. The only way to catch this physiological behavior is to couple the arteries with a model of heart, or at least a model of left ventricle.

A constitutive law for the myocardium, controlled by an electrical command, has been developed in the CardioSense3D project [0]. One of our objectives is to couple artery models with this heart model.

A long term goal is to achieve 3D simulations of a system including heart and arteries. One of the difficulties of this very challenging task is to model the cardiac valves. To this purpose, we investigate a mix of arbitrary Lagrangian Eulerian and fictitious domain approaches or x-fem strategies, or simplified valve models based on an immersed surface strategy.

[0] http://www-sop.inria.fr/CardioSense3D/

3.2.2. Heart perfusion modeling

The heart is the organ that regulates, through its periodical contraction, the distribution of oxygenated blood in human vessels in order to nourish the different parts of the body. The heart needs its own supply of blood to work. The coronary arteries are the vessels that accomplish this task. The phenomenon by which blood reaches myocardial heart tissue starting from the blood vessels is called in medicine perfusion. The analysis of heart perfusion is an interesting and challenging problem. Our aim is to perform a three-dimensional dynamical numerical simulation of perfusion in the beating heart, in order to better understand the phenomena linked to perfusion. In particular the role of the ventricle contraction on the perfusion of the heart is investigated as well as the influence of blood on the solid mechanics of the ventricle. Heart perfusion in fact implies the interaction between heart muscle and blood vessels, in a sponge-like material that contracts at every heartbeat via the myocardium fibers.

Despite recent advances on the anatomical description and measurements of the coronary tree and on the corresponding physiological, physical and numerical modeling aspects, the complete modeling and simulation of blood flows inside the large and the many small vessels feeding the heart is still out of reach. Therefore, in order to model blood perfusion in the cardiac tissue, we must limit the description of the detailed flows at a given space scale, and simplify the modeling of the smaller scale flows by aggregating these phenomena into macroscopic quantities, by some kind of “homogenization” procedure. To that purpose, the modeling of the fluid-solid coupling within the framework of porous media appears appropriate.

Poromechanics is a simplified mixture theory where a complex fluid-structure interaction problem is replaced by a superposition of both components, each of them representing a fraction of the complete material at every point. It originally emerged in soils mechanics with the work of Terzaghi [63], and Biot [55] later gave a description of the mechanical behavior of a porous medium using an elastic formulation for the solid matrix, and Darcy’s law for the fluid flow through the matrix. Finite strain poroelastic models have been proposed (see references in [56]), albeit with *ad hoc* formulations for which compatibility with thermodynamics laws and incompressibility conditions is not established.

3.2.3. Tumor and vascularization

The same way the myocardium needs to be perfused for the heart to beat, when it has reached a certain size, tumor tissue needs to be perfused by enough blood to grow. It thus triggers the creation of new blood vessels (angiogenesis) to continue to grow. The interaction of tumor and its micro-environment is an active field of research. One of the challenges is that phenomena (tumor cell proliferation and death, blood vessel adaptation, nutrient transport and diffusion, etc) occur at different scales. A multi-scale approach is thus being developed to tackle this issue. The long term objective is to predict the efficiency of drugs and optimize therapy of cancer.

3.2.4. Respiratory tract modeling

We aim at developing a multiscale model of the respiratory tract. Intraprenchymal airways distal from generation 7 of the tracheabronchial tree (TBT), which cannot be visualized by common medical imaging techniques, are modeled either by a single simple model or by a model set according to their order in TBT. The single model is based on straight pipe fully developed flow (Poiseuille flow in steady regimes) with given alveolar pressure at the end of each compartment. It will provide boundary conditions at the bronchial ends of 3D TBT reconstructed from imaging data. The model set includes three serial models. The generation down to the pulmonary lobule will be modeled by reduced basis elements. The lobular airways will be represented by a fractal homogenization approach. The alveoli, which are the gas exchange loci between blood and inhaled air, inflating during inspiration and deflating during expiration, will be described by multiphysics homogenization.

SERENA Team

3. Research Program

3.1. Multiphysics coupling

Within our project, we start from the conception and analysis of *models* based on *partial differential equations* (PDEs). Already at the PDE level, we address the question of *coupling* of different models; examples are that of simultaneous fluid flow in a discrete network of two-dimensional *fractures* and in the surrounding three-dimensional porous medium, or that of interaction of a compressible flow with the surrounding elastic *deformable structure*. The key physical characteristics need to be captured, whereas existence, uniqueness, and continuous dependence on the data are minimal analytic requirements that we seek to satisfy. At the modeling stage, we also develop model-order reduction techniques, such as the use of reduced basis techniques or proper generalized decompositions, to tackle evolutive problems, in particular in the nonlinear case.

3.2. Structure-preserving discretizations and discrete element methods

We consequently design *numerical methods* for the devised model. Traditionally, we have worked in the context of finite element, finite volume, mixed finite element, and discontinuous Galerkin methods. Novel classes of schemes enable the use of general *polygonal* and *polyhedral meshes* with *nonmatching interfaces*, and we develop them in response to a high demand from our industrial partners (namely EDF and IFP Energies Nouvelles). Our requirement is to derive *structure-preserving* methods, i.e., methods that mimic at the discrete level fundamental properties of the underlying PDEs, such as conservation principles and preservation of invariants. Here, the theoretical questions are closely linked to *differential geometry* for the lowest-order schemes. For the schemes we develop, we study existence, uniqueness, and stability questions, and derive a priori convergence estimates. Our special interest is in higher-order methods like the hybrid high-order method, which have recently begun to receive significant attention. Even though their use in practice may not be immediate, we believe that they represent the future generation of numerical methods for industrial simulations.

3.3. Domain decomposition and Newton–Krylov (multigrid) solvers

We next concentrate an intensive effort on the development and analysis of efficient solvers for the systems of nonlinear algebraic equations that result from the above discretizations. We have in the past developed *Newton–Krylov solvers* like the adaptive inexact Newton method, and we place a particular emphasis on *parallelization* achieved via the *domain decomposition* method. Here we traditionally specialize in *Robin transmission conditions*, where an optimized choice of the parameter has already shown speed-ups in orders of magnitude in terms of the number of domain decomposition iterations in model cases. We concentrate in the SERENA project on adaptation of these algorithms to the above novel discretization schemes, on the optimization of the free Robin parameter for challenging situations, and also on the use of the Ventcell transmission conditions. Another feature is the use of such algorithms in time-dependent problems in *space-time* domain decomposition that we have recently pioneered. This allows the use of different time steps in different parts of the computational domain and turns out to be particularly useful in porous media applications, where the amount of diffusion (permeability) varies abruptly, so that the evolution speed varies significantly from one part of the computational domain to another. Our new theme here are *Newton–multigrid solvers*, where the geometric multigrid solver is *tailored* to the specific problem under consideration and to the specific numerical method, with problem- and discretization-dependent restriction, prolongation, and smoothing. This in particular yields mass balance at each iteration step, a highly demanded feature in most of the target applications. The solver itself is then *adaptively steered* at each execution step by an a posteriori error estimate.

3.4. Reliability by a posteriori error control

The fourth part of our theoretical efforts goes towards guaranteeing the results obtained at the end of the numerical simulation. Here a key ingredient is the development of rigorous *a posteriori estimates* that make it possible to estimate in a fully computable way the error between the unknown exact solution and its numerical approximation. Our estimates also allow to distinguish the different *components* of the overall *error*, namely the errors coming from modeling, from the discretization scheme, from the nonlinear (Newton) solver, and from the linear algebraic (Krylov, domain decomposition, multigrid) solver. A new concept here is that of *local stopping criteria*, where all the error components are balanced locally within each computational mesh element. This naturally connects all parts of the numerical simulation process and gives rise to novel *fully adaptive algorithms*. We shall then address theoretically the question of convergence of the new algorithms and prove their numerical quasi-optimality, meaning that they need, up to a generic constant, the smallest possible number of degrees of freedom to achieve the given accuracy. We in particular seek to prove a guaranteed error reduction in terms of the number of degrees of freedom.

3.5. Safe and correct programming

Finally, we concentrate on the issue of computer implementation of scientific computing programs. Increasing complexity of algorithms for modern scientific computing makes it a major challenge to implement them in the traditional imperative languages popular in the community. As an alternative, the computer science community provides theoretically sound tools for *safe* and *correct programming*. We explore here the use of these tools to design generic solutions for the implementation of the class of scientific computing software that we deal with. Our focus ranges from high-level programming via *functional programming* with OCAML through safe and easy parallelism via *skeleton parallel programming* with SKLML to proofs of correctness of numerical algorithms and programs via *mechanical proofs* with COQ.

SERPICO Project-Team

3. Research Program

3.1. Statistics and algorithms for computational microscopy

Many live-cell fluorescence imaging experiments are limited in time to prevent phototoxicity and photobleaching. The amount of light and time required to observe entire cell divisions can generate biological artifacts. In order to produce images compatible with the dynamic processes in living cells as seen in video-microscopy, we study the potential of denoising, superresolution, tracking, and motion analysis methods in the Bayesian and the robust statistics framework to extract information and to improve image resolution while preserving cell integrity.

In this area, we have already demonstrated that image denoising allows images to be taken more frequently or over a longer period of time [6]. The major advantage is to preserve cell integrity over time since spatio-temporal information can be restored using computational methods [9], [3], [10], [5]. This idea has been successfully applied to wide-field, spinning-disk confocal microscopy [2], TIRF [40], fast live imaging and 3D-PALM using the OMX system in collaboration with J. Sedat and M. Gustafsson at UCSF [6]. The corresponding ND-SAFIR denoiser software (see Section 6.7) has been licensed to a large set of laboratories over the world. New information restoration and image denoising methods are currently investigated to make SIM imaging compatible with the imaging of molecular dynamics in live cells. Unlike other optical sub-diffraction limited techniques (e.g. STED [51], PALM [41]) SIM has the strong advantage of versatility when considering the photo-physical properties of the fluorescent probes [49]. Such developments are also required to be compatible with “high-throughput microscopy” since several hundreds of cells are observed at the same time and the exposure times are typically reduced.

3.2. From image data to descriptors: dynamic analysis and trajectory computation

3.2.1. Motion analysis and tracking

The main challenge is to detect and track xFP tags with high precision in movies representing several Giga-Bytes of image data. The data are most often collected and processed automatically to generate information on partial or complete trajectories. Accordingly, we address both the methodological and computational issues involved in object detection and multiple objects tracking in order to better quantify motion in cell biology. Classical tracking methods have limitations as the number of objects and clutter increase. It is necessary to correctly associate measurements with tracked objects, i.e. to solve the difficult data association problem [57]. Data association even combined with sophisticated particle filtering techniques [60] or matching techniques [58] is problematic when tracking several hundreds of similar objects with variable velocities. Developing new optical flow and robust tracking methods and models in this area is then very stimulating since the problems we have to solve are really challenging and new for applied mathematics. In motion analysis, the goal is to formulate the problem of optical flow estimations in ways that take physical causes of brightness constancy violations into account [46], [50]. The interpretation of computed flow fields enables to provide spatio-temporal signatures of particular dynamic processes (e.g. Brownian and directed motion) and could help to complete the traffic modelling.

3.2.2. Event detection and motion classification

Protein complexes in living cells undergo multiple states of local concentration or dissociation, sometimes associated with diffusion processes. These events can be observed at the plasma membrane with TIRF microscopy. The difficulty arises when it becomes necessary to distinguish continuous motions due to trafficking from sudden events due to molecule concentrations or their dissociations. Typically, plasma membrane vesicle docking, membrane coat constitution or vesicle endocytosis are related to these issues.

Several approaches can be considered for the automatic detection of appearing and vanishing particles (or spots) in wide-field and TIRF microscopy images. Ideally this could be performed by tracking all the vesicles contained in the cell [60], [48]. Among the methods proposed to detect particles in microscopy images [61], [59], none is dedicated to the detection of a small number of particles appearing or disappearing suddenly between two time steps. Our way of handling small blob appearances/dis-appearances originates from the observation that two successive images are redundant and that occlusions correspond to blobs in one image which cannot be reconstructed from the other image [2] (see also [44]). Furthermore, recognizing dynamic protein behaviors in live cell fluorescence microscopy is of paramount importance to understand cell mechanisms. In our studies, it is challenging to classify intermingled dynamics of vesicular movements, docking/tethering, and ultimately, plasma membrane fusion of vesicles that leads to membrane diffusion or exocytosis of cargo proteins. Our aim is then to model, detect, estimate and classify subcellular dynamic events in TIRF microscopy image sequences. We investigate methods that exploits space-time information extracted from a couple of successive images to classify several types of motion (directed, diffusive (or Brownian) and confined motion) or compound motion.

3.3. From models to image data: simulation and modelling of membrane transport

Mathematical biology is a field in expansion, which has evolved into various branches and paradigms to address problems at various scales ranging from ecology to molecular structures. Nowadays, system biology [52], [63] aims at modelling systems as a whole in an integrative perspective instead of focusing on independent biophysical processes. One of the goals of these approaches is the cell in silico as investigated at Harvard Medical School (http://vcp.med.harvard.edu/) or the VCell of the University of Connecticut Health Center (http://www.nrcam.uchc.edu/). Previous simulation-based methods have been investigated to explain the spatial organization of microtubules [53] but the method is not integrative and a single scale is used to describe the visual patterns. In this line of work, we propose several contributions to combine imaging, traffic and membrane transport modelling in cell biology.

In this area, we focus on the analysis of transport intermediates (vesicles) that deliver cellular components to appropriate places within cells. We have already investigated the concept of Network Tomography (NT) [62] mainly developed for internet traffic estimation. The idea is to determine mean traffic intensities based on statistics accumulated over a period of time. The measurements are usually the number of vesicles detected at each destination region receiver. The NT concept has been investigated also for simulation [4] since it can be used to statistically mimic the contents of real traffic image sequences. In the future, we plan to incorporate more prior knowledge on dynamics to improve representation. An important challenge is to correlate stochastic, dynamical, one-dimensional *in silico* models studied at the nano-scale in biophysics, to 3D images acquired in vivo at the scale of few hundred nanometers.

SISTM Project-Team

3. Research Program

3.1. Mecanistic modelling

When studying the dynamics of a given marker, say the HIV concentration in the blood (HIV viral load), one can for instance use descriptive models summarising the dynamics over time in term of slopes of the trajectories [51]. These slopes can be compared between treatment groups or according to patients' characteristics. Another way for analysing these data is to define a mathematical model based on the biological knowledge of what drives HIV dynamics. In this case, it is mainly the availability of target cells (the CD4+ T lymphocytes), the production and death rates of infected cells and the clearance of the viral particles that impact the dynamics. Then, a mathematical model most often based on ordinary differential equations (ODE) can be written [41]. Estimating the parameters of this model to fit observed HIV viral load gave a crucial insight in HIV pathogenesis as it revealed the very short half-life of the virions and infected cells and therefore a very high turnover of the virus, making mutations a very frequent event [40].

Having a good mechanistic model in a biomedical context such as HIV infection opens doors to various applications beyond a good understanding of the data. Global and individual predictions can be excellent because of the external validity of a model based on main biological mechanisms. Control theory may serve for defining optimal interventions or optimal designs to evaluate new interventions [30]. Finally, these models can capture explicitly the complex relationship between several processes that change over time and may therefore challenge other proposed approaches such as marginal structural models to deal with causal associations in epidemiology [28].

Therefore, we postulate that this type of model could be very useful in the context of our research that is in complex biological systems. The definition of the model needs to identify the parameter values that fit the data. In clinical research this is challenging because data are sparse, and often unbalanced, coming from populations of subjects. A substantial inter-individual variability is always present and needs to be accounted as this is the main source of information. Although many approaches have been developed to estimate the parameters of non-linear mixed models [44], [54], [33], [42], [36], [53], the difficulty associated with the complexity of ODE models and the sparsity of the data leading to identifiability issues need further research.

3.2. High dimensional data

With the availability of omics data such as genomics (DNA), transcriptomics (RNA) or proteomics (proteins), but also other types of data, such as those arising from the combination of large observational databases (e.g. in pharmacoepidemiology or environmental epidemiology), high-dimensional data have became increasingly common. Use of molecular biological technics such as Polymerase Chain Reaction (PCR) allows for amplification of DNA or RNA sequences. Nowadays, microarray and Next Generation Sequencing (NGS) techniques give the possibility to explore very large portions of the genome. Furthermore, other assays have also evolved, and traditional measures such as cytometry or imaging have became new sources of big data. Therefore, in the context of HIV research, the dimension of the datasets has much grown in term of number of variables per individual than in term of number of included patients although this latter is also growing thanks to the multi-cohort collaborations such as CASCADE or COHERE organized in the EuroCoord network [0]. As an exemple, in a recent phase 1/2 clinical trial evaluating the safety and the immunological response to a dendritic cell-based HIV vaccine, 19 infected patients were included. Bringing together data on cell count, cytokine production, gene expression and viral genome change led to a 20 Go database [50]. This is far from big databases faced in other areas but constitutes a revolution in clinical research where clinical trials of hundred of patients sized few hundred of Ko at most. Therefore, more than the storage and calculation capacities, the challenge is the comprehensive analysis of these datasets.

[0] see online at http://www.eurocoord.net

The objective is either to select the relevant information or to summarize it for understanding or prediction purposes. When dealing with high dimensional data, the methodological challenge arises from the fact that datasets typically contain many variables, much more than observations. Hence, multiple testing is an obvious issue that needs to be taken into account [45]. Furthermore, conventional methods, such as linear models, are inefficient and most of the time even inapplicable. Specific methods have been developed, often derived from the machine learning field, such as regularization methods [52]. The integrative analysis of large datasets is challenging. For instance, one may want to look at the correlation between two large scale matrices composed by the transcriptome in the one hand and the proteome on the other hand [37]. The comprehensive analysis of these large datasets concerning several levels from molecular pathways to clinical response of a population of patients needs specific approaches and a very close collaboration with the providers of data that is the immunologists, the virologists, the clinicians...

STEEP Project-Team

3. Research Program

3.1. Development of numerical systemic models (economy / society /environment) at local scales

The problem we consider is intrinsically interdisciplinary: it draws on social sciences, ecology or science of the planet. The modeling of the considered phenomena must take into account many factors of different nature which interact with varied functional relationships. These heterogeneous dynamics are *a priori* nonlinear and complex: they may have saturation mechanisms, threshold effects, and may be density dependent. The difficulties are compounded by the strong interconnections of the system (presence of important feedback loops) and multi-scale spatial interactions. Environmental and social phenomena are indeed constrained by the geometry of the area in which they occur. Climate and urbanization are typical examples. These spatial processes involve proximity relationships and neighborhoods, like for example, between two adjacent parcels of land, or between several macroscopic levels of a social organization. The multi-scale issues are due to the simultaneous consideration in the modeling of actors of different types and that operate at specific scales (spatial and temporal). For example, to properly address biodiversity issues, the scale at which we must consider the evolution of rurality is probably very different from the one at which we model the biological phenomena.

In this context, to develop flexible integrated systemic models (upgradable, modular, ...) which are efficient, realistic and easy to use (for developers, modelers and end users) is a challenge in itself. What mathematical representations and what computational tools to use? Nowadays many tools are used: for example, cellular automata (e.g. in the LEAM model), agent models (e.g. URBANSIM), system dynamics (e.g. World3), large systems of ordinary equations (e.g. equilibrium models such as TRANUS), and so on. Each of these tools has strengths and weaknesses. Is it necessary to invent other representations? What is the relevant level of modularity? How to get very modular models while keeping them very coherent and easy to calibrate? Is it preferable to use the same modeling tools for the whole system, or can we freely change the representation for each considered subsystem? How to easily and effectively manage different scales? (difficulty appearing in particular during the calibration process). How to get models which automatically adapt to the granularity of the data and which are always numerically stable? (this has also a direct link with the calibration processes and the propagation of uncertainties). How to develop models that can be calibrated with reasonable efforts, consistent with the (human and material) resources of the agencies and consulting firms that use them?

Before describing our research axes, we provide a brief overview of the types of models that we are or will be working with. As for LUTI (Land Use and Transportation Integrated) modeling, we have been using the TRANUS model since the start of our group. It is the most widely used LUTI model, has been developed since 1982 by the company Modelistica, and is distributed *via* Open Source software. TRANUS proceeds by solving a system of deterministic nonlinear equations and inequalities containing a number of economic parameters (e.g. demand elasticity parameters, location dispersion parameters, etc.). The solution of such a system represents an economic equilibrium between supply and demand. A second LUTI model that will be considered in the near future, within the CITiES project, is UrbanSim [0]. Whereas TRANUS aggregates over e.g. entire population or housing categories, UrbanSim takes a micro-simulation approach, modeling and simulating choices made at the level of individual households, businesses, and jobs, for instance, and it operates on a finer geographic scale than TRANUS.

[0] http://www.urbansim.org

On the other hand, the scientific domains related to ecosystem services and ecological accounting are much less mature than the one of urban economy from a modelling point of view (as a consequence of our more limited knowledge of the relevant complex processes and/or more limited available data). Nowadays, the community working on ecological accounting develops statistical models based on the enforcement of the mass conservation constraint for accounting for material fluxes through a territorial unit or a supply chain, relying on more or less simple data correlations when the relevant data is missing; the overall modelling makes heavy use of more or less sophisticated linear algebra and constrained optimization techniques. The ecosystem service community has been using statical models too, but is also developing more sophisticated models based for example on system dynamics, multi-agent type simulations or cellular models. In the ESNET project, STEEP will work in particular on a land use/ land cover change (LUCC) modelling environments (Dinamica [0]) which belongs to the category of spatially explicit statistical models.

In the following, our two main research axes are described, from the point of view of applied mathematical development. The domains of application of this research effort is described in the application section, where some details about the context of each field is given.

3.2. Model calibration and validation

The overall calibration of the parameters that drive the equations implemented in the above models is a vital step. Theoretically, as the implemented equations describe e.g. socio-economic phenomena, some of these parameters should in principle be accurately estimated from past data using econometrics and statistical methods like regressions or maximum likelihood estimates, e.g. for the parameters of logit models describing the residential choices of households. However, this theoretical consideration is often not efficient in practice for at least two main reasons. First, the above models consist of several interacting modules. Currently, these modules are typically calibrated independently; this is clearly sub-optimal as results will differ from those obtained after a global calibration of the interaction system, which is the actual final objective of a calibration procedure. Second, the lack of data is an inherent problem.

As a consequence, models are usually calibrated by hand. The calibration can typically take up to 6 months for a medium size LUTI model (about 100 geographic zones, about 10 sectors including economic sectors, population and employment categories). This clearly emphasizes the need to further investigate and at least semi-automate the calibration process. Yet, in all domains STEEP considers, very few studies have addressed this central issue, not to mention calibration under uncertainty which has largely been ignored (with the exception of a few uncertainty propagation analyses reported in the literature).

Besides uncertainty analysis, another main aspect of calibration is numerical optimization. The general state-of-the-art on optimization procedures is extremely large and mature, covering many different types of optimization problems, in terms of size (number of parameters and data) and type of cost function(s) and constraints. Depending on the characteristics of the considered models in terms of dimension, data availability and quality, deterministic or stochastic methods will be implemented. For the former, due to the presence of non-differentiability, it is likely, depending on their severity, that derivative free control methods will have to be preferred. For the latter, particle-based filtering techniques and/or metamodel-based optimization techniques (also called response surfaces or surrogate models) are good candidates.

These methods will be validated, by performing a series of tests to verify that the optimization algorithms are efficient in the sense that 1) they converge after an acceptable computing time, 2) they are robust and 3) that the algorithms do what they are actually meant to. For the latter, the procedure for this algorithmic validation phase will be to measure the quality of the results obtained after the calibration, i.e. we have to analyze if the calibrated model fits sufficiently well the data according to predetermined criteria.

To summarize, the overall goal of this research axis is to address two major issues related to calibration and validation of models: (a) defining a calibration methodology and developing relevant and efficient algorithms to facilitate the parameter estimation of considered models; (b) defining a validation methodology and developing the related algorithms (this is complemented by sensitivity analysis, see the following section).

[0] http://www.csr.ufmg.br/dinamica/

In both cases, analyzing the uncertainty that may arise either from the data or the underlying equations, and quantifying how these uncertainties propagate in the model, are of major importance. We will work on all those issues for the models of all the applied domains covered by STEEP.

3.3. Sensitivity analysis

A sensitivity analysis (SA) consists, in a nutshell, in studying how the uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model inputs. It is complementary to an uncertainty analysis, which focuses on quantifying uncertainty in model output. SA's can be useful for several purposes, such as guiding model development and identifying the most influential model parameters and critical data items. Identifying influential model parameters may help in divising metamodels (or, surrogate models) that approximate an original model and may be simulated, calibrated, or analyzed more efficiently. As for detecting critical data items, this may indicate for which type of data more effort must be spent in the data collection process in order to eventually improve the model's reliability. Finally, SA can be used as one means for validating models, together with validation based on historical data (or, put simply, using training and test data) and validation of model parameters and outputs by experts in the respective application area. All these uses of SA will be considered in our research.

The first two applications of SA are linked to model calibration, discussed in the previous section. Indeed, prior to the development of the calibration tools, one important step is to select the significant or sensitive parameters and to evaluate the robustness of the calibration results with respect to data noise (stability studies). This may be performed through a global sensitivity analysis, e.g. by computation of Sobol's indices. Many problems will have to be circumvented e.g. difficulties arising from dependencies of input variables, variables that obey a spatial organization, or switch inputs. We will take up on current work in the statistics community on SA for these difficult cases.

As for the third application of SA, model validation, a preliminary task bears on the propagation of uncertainties. Identifying the sources of uncertainties and their nature is crucial to propagate them via Monte Carlo techniques. To make a Monte Carlo approach computationally feasible, it is necessary to develop specific metamodels. Both the identification of the uncertainties and their propagation require a detailed knowledge of the data collection process; these are mandatory steps before a validation procedure based on SA can be implemented. First, we will focus on validating LUTI models, starting with the CITiES ANR project: here, an SA consists in defining various land use policies and transportation scenarios and in using these scenarios to test the integrated land use and transportation model. Current approaches for validation by SA consider several scenarios and propose various indicators to measure the simulated changes. We will work towards using sensitivity indices based on functional analysis of variance, which will allow us to compare the influence of various inputs on the indicators. For example it will allow the comparison of the influences of transportation and land use policies on several indicators.

TAPDANCE Team

3. Research Program

3.1. Ongoing work

Recent theoretical work (Meunier, Woods "The non-cooperative tile assembly model is not intrinsically universal or capable of bounded Turing machine simulation") to be published in 2017 by has centered on the power of a model of self-assembly. In this model, called the noncooperative (or temperature 1) abstract Tile Assembly Model, square tiles assemble structures, called assemblies, in the discrete plane where each tile binds to a growing structure if one of its 4 coloured edges matches the colour of some available site on a growing assembly. It has been conjectured since 2000 that this model is not capable of computation or other sophisticated forms of growth. We show two results. One of our results states that time-bounded Turing machine computation is impossible in this model if we require the simulation to occur in a bounded rectangle in the plane. This result has a short proof that essentially follows from our other main result which states that this model is not "intrinsically universal". This latter result means that there is no single tileset in this model that can simulate any instance of the model, answering a question from and contrasting a result for the more general cooperative (temperature 2) model.

Other work by Woods has focused on experimentally implementing a wide class of Boolean circuits of a certain form. Experiments were mostly carried out at Caltech, and the work is in collaboration with colleagues at Caltech, UC Davis, Harvard and Cambridge and a publication is in preparation with [Woods, Doty, Myhrvold, Hui, Zhou, Yin, Winfree]. Details will be described in a future report subsequent to publication.

Work published earlier in 2016 (Erik D Demaine, Matthew J Patitz, Trent A Rogers, Robert T Schweller Scott M Summers and Damien Woods, "The two-handed tile assembly model is not intrinsically universal", Algorithmica 74:2, pages 812–850 (2016). not on HAL) shows results on a hierarchal model of algorithmic self-assembly called the two-handed self-assembly model (2HAM). Specifically, that the model is not intrinsically universal. In fact, we show that for all $\tau' < \tau$, each temperature-τ' 2HAM tile system does not simulate at least one temperature-τ 2HAM tile system. This impossibility result proves that the 2HAM is not intrinsically universal and stands in contrast to the fact that the (single-tile addition) abstract Tile Assembly Model is intrinsically universal. On the positive side, we prove that, for every fixed temperature $\tau \geq 2$, temperature-τ 2HAM tile systems are indeed intrinsically universal. In other words, for each τ there is a single intrinsically universal 2HAM tile set U_τ that, when appropriately initialized, is capable of simulating the behavior of any temperature-τ 2HAM tile system. As a corollary, we find an infinite set of infinite hierarchies of 2HAM systems with strictly increasing simulation power within each hierarchy. Finally, we show that for each τ , there is a temperature-τ 2HAM system that simultaneously simulates all temperature-τ 2HAM systems.

There are a number of projects being designed along the lines of topics above in Overall Objectives.

TONUS Team

3. Research Program

3.1. Kinetic models for plasmas

The fundamental model for plasma physics is the coupled Vlasov-Maxwell kinetic model: the Vlasov equation describes the distribution function of particles (ions and electrons), while the Maxwell equations describe the electromagnetic field. In some applications, it may be necessary to take into account relativistic particles, which lead to consider the relativistic Vlasov equation, but generally, tokamak plasmas are supposed to be non relativistic. The distribution function of particles depends on seven variables (three for space, three for velocity and one for time), which yields a huge amount of computations.

To these equations we must add several types of source terms and boundary conditions for representing the walls of the tokamak, the applied electromagnetic field that confines the plasma, fuel injection, collision effects, etc.

Tokamak plasmas possess particular features, which require developing specialized theoretical and numerical tools.

Because the magnetic field is strong, the particle trajectories have a very fast rotation around the magnetic field lines. A full resolution would require prohibitive amount of calculations. It is then necessary to develop models where the cyclotron frequency tends to infinity in order to obtain tractable calculations. The resulting model is called a gyrokinetic model. It allows us to reduce the dimensionality of the problem. Such models are implemented in GYSELA and Selalib. Those models require averaging of the acting fields during a rotation period along the trajectories of the particles. This averaging is called the gyroaverage and requires specific discretizations.

The tokamak and its magnetics fields present a very particular geometry. Some authors have proposed to return to the intrinsic geometrical versions of the Vlasov-Maxwell system in order to build better gyrokinetic models and adapted numerical schemes. This implies the use of sophisticated tools of differential geometry: differential forms, symplectic manifolds, and Hamiltonian geometry.

In addition to theoretical modeling tools, it is necessary to develop numerical schemes adapted to kinetic and gyrokinetic models. Three kinds of methods are studied in TONUS: Particle-In-Cell (PIC) methods, semi-Lagrangian and fully Eulerian approaches.

3.1.1. Gyrokinetic models: theory and approximation

In most phenomena where oscillations are present, we can establish a three-model hierarchy: (i) the model parameterized by the oscillation period, (ii) the limit model and (iii) the two-scale model, possibly with its corrector. In a context where one wishes to simulate such a phenomenon where the oscillation period is small and where the oscillation amplitude is not small, it is important to have numerical methods based on an approximation of the Two-Scale model. If the oscillation period varies significantly over the domain of simulation, it is important to have numerical methods that approximate properly and effectively the model parameterized by the oscillation period and the Two-Scale model. Implemented Two-Scale Numerical Methods (for instance by Frénod et al. [20]) are based on the numerical approximation of the Two-Scale model. These are called of order 0. A Two-Scale Numerical Method is called of order 1 if it incorporates information from the corrector and from the equation of which this corrector is a solution. If the oscillation period varies between very small values and values of order 1, it is necessary to have new types of numerical schemes (Two-Scale Asymptotic Preserving Schemes of order 1 or TSAPS) with the property of being able to preserve the asymptotics between the model parameterized by the oscillation period and the Two-Scale model with its corrector. A first work in this direction has been initiated by Crouseilles et al. [18].

3.1.2. Semi-Lagrangian schemes

The Strasbourg team has a long and recognized experience in numerical methods of Vlasov-type equations. We are specialized in both particle and phase space solvers for the Vlasov equation: Particle-in-Cell (PIC) methods and semi-Lagrangian methods. We also have a longstanding collaboration with the CEA of Cadarache for the development of the GYSELA software for gyrokinetic tokamak plasmas.

The Vlasov and the gyrokinetic models are partial differential equations that express the transport of the distribution function in the phase space. In the original Vlasov case, the phase space is the six-dimension position-velocity space. For the gyrokinetic model, the phase space is five-dimensional because we consider only the parallel velocity in the direction of the magnetic field and the gyrokinetic angular velocity instead of three velocity components.

A few years ago, Eric Sonnendrücker and his collaborators introduced a new family of methods for solving transport equations in the phase space. This family of methods are the semi-Lagrangian methods. The principle of these methods is to solve the equation on a grid of the phase space. The grid points are transported with the flow of the transport equation for a time step and interpolated back periodically onto the initial grid. The method is then a mix of particle Lagrangian methods and Eulerian methods. The characteristics can be solved forward or backward in time leading to the Forward Semi-Lagrangian (FSL) or Backward Semi-Lagrangian (BSL) schemes. Conservative schemes based on this idea can be developed and are called Conservative Semi-Lagrangian (CSL).

GYSELA is a 5D full gyrokinetic code based on a classical backward semi-Lagrangian scheme (BSL) [27] for the simulation of core turbulence that has been developed at CEA Cadarache in collaboration with our team [21]. Although GYSELA was carefully developed to be conservative at lowest order, it is not exactly conservative, which might be an issue when the simulation is under-resolved, which always happens in turbulence simulations due to the formation of vortices which roll up.

3.1.3. PIC methods

Historically PIC methods have been very popular for solving the Vlasov equations. They allow solving the equations in the phase space at a relatively low cost. The main disadvantage of the method is that, due to its random aspect, it produces an important numerical noise that has to be controlled in some way, for instance by regularizations of the particles, or by divergence correction techniques in the Maxwell solver. We have a longstanding experience in PIC methods and we started implement them in Selalib. An important aspect is to adapt the method to new multicore computers. See the work by Crestetto and Helluy [17].

3.2. Reduced kinetic models for plasmas

As already said, kinetic plasmas computer simulations are very intensive, because of the gyrokinetic turbulence. In some situations, it is possible to make assumptions on the shape of the distribution function that simplify the model. We obtain in this way a family of fluid or reduced models.

Assuming that the distribution function has a Maxwellian shape, for instance, we obtain the MagnetoHydroDynamic (MHD) model. It is physically valid only in some parts of the tokamak (at the edges for instance). The fluid model is generally obtained from the hypothesis that the collisions between particles are strong. Fine collision models are mainly investigated by other partners of the IPL (Inria Project Lab) FRATRES. In our approach we do not assume that the collisions are strong, but rather try to adapt the representation of the distribution function according to its shape, keeping the kinetic effects. The reduction is not necessarily a consequence of collisional effects. Indeed, even without collisions, the plasma may still relax to an equilibrium state over sufficiently long time scales (Landau damping effect). Recently, a team at the Plasma Physics Institut (IPP) in Garching has carried out a statistical analysis of the 5D distribution functions obtained from gyrokinetic tokamak simulations [22]. They discovered that the fluctuations are much higher in the space directions than in the velocity directions (see Figure 1).

This indicates that the approximation of the distribution function could require fewer data while still achieving a good representation, even in the collisionless regime.

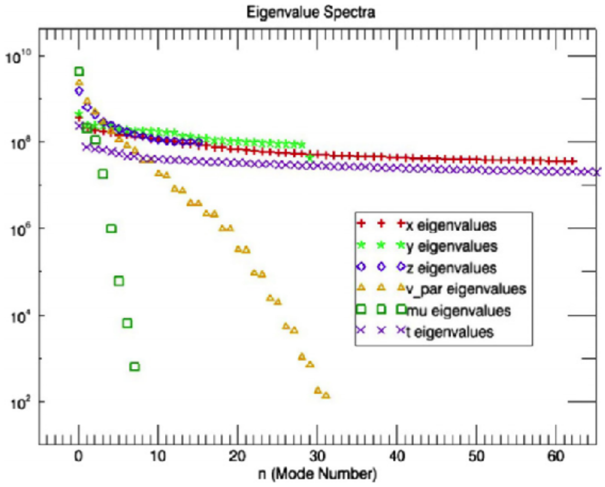

Figure 1. Space and velocity fluctuations spectra (from [22])

Our approach is different from the fluid approximation. In what follows we call this the "reduced model" approach. A reduced model is a model where the explicit dependency on the velocity variable is removed. In a more mathematical way, we consider that in some regions of the plasma, it is possible to exhibit a (preferably small) set of parameters α that allows us to describe the main properties of the plasma with a generalized "Maxwellian" M. Then

$$f(x,v,t)=M(\alpha(x,t),v).$$

In this case it is sufficient to solve for $\alpha(x,t)$. Generally, the vector α is solution of a first order hyperbolic system.

Several approaches are possible: waterbag approximations, velocity space transforms, *etc.*

3.2.1. Velocity space transformations

An experiment made in the 60's [25] exhibits in a spectacular way the reversible nature of the Vlasov equations. When two perturbations are applied to a plasma at different times, at first the plasma seems to damp and reach an equilibrium. But the information of the perturbations is still here and "hidden" in the high frequency microscopic oscillations of the distribution function. At a later time a resonance occurs and the plasma produces an echo. The time at which the echo occurs can be computed (see Villani [0], page 74). The fine mathematical study of this phenomenon allowed C. Villani and C. Mouhot to prove their famous result on the rigorous nonlinear Landau damping [26].

More practically, this experiment and its theoretical framework show that it is interesting to represent the distribution function by an expansion on an orthonormal basis of oscillating functions in the velocity variables. This representation allows a better control of the energy transfer between the low frequencies and the high frequencies in the velocity direction, and thus provides more relevant numerical methods. This kind of approach is studied for instance by Eliasson in [19] with the Fourier expansion.

[0] Landau damping. CEMRACS 2010 lectures. http://smai.emath.fr/cemracs/cemracs10/PROJ/Villani-lectures.pdf

In long time scales, filamentation phenomena result in high frequency oscillations in velocity space that numerical schemes cannot resolve. For stability purposes, most numerical schemes contain dissipation mechanisms that may affect the precision of the finest oscillations that can be resolved.

3.2.2. Adaptive modeling

Another trend in scientific computing is to optimize the computation time through adaptive modeling. This approach consists in applying the more efficient model locally, in the computational domain, according to an error indicator. In tokamak simulations, this kind of approach could be very efficient, if we are able to choose locally the best intermediate kinetic-fluid model as the computation runs. This field of research is very promising. It requires developing a clever hierarchy of models, rigorous error indicators, versatile software architecture, and algorithms adapted to new multicore computers.

3.2.3. Numerical schemes

As previously indicated, an efficient method for solving the reduced models is the Discontinuous Galerkin (DG) approach. It is possible to make it of arbitrary order. It requires limiters when it is applied to nonlinear PDEs occurring for instance in fluid mechanics. But the reduced models that we intent to write are essentially linear. The nonlinearity is concentrated in a few coupling source terms.

In addition, this method, when written in a special set of variables, called the entropy variables, has nice properties concerning the entropy dissipation of the model. It opens the door to constructing numerical schemes with good conservation properties and no entropy dissipation, as already used for other systems of PDEs [28], [16], [24], [23].

3.3. Electromagnetic solvers

A precise resolution of the electromagnetic fields is essential for proper plasma simulation. Thus it is important to use efficient solvers for the Maxwell systems and its asymptotics: Poisson equation and magnetostatics.

The proper coupling of the electromagnetic solver with the Vlasov solver is also crucial for ensuring conservation properties and stability of the simulation.

Finally plasma physics implies very different time scales. It is thus very important to develop implicit Maxwell solvers and Asymptotic Preserving (AP) schemes in order to obtain good behavior on long time scales.

3.3.1. Coupling

The coupling of the Maxwell equations to the Vlasov solver requires some precautions. The most important is to control the charge conservation errors, which are related to the divergence conditions on the electric and magnetic fields. We will generally use divergence correction tools for hyperbolic systems presented for instance in [15] (and included references).

3.3.2. Implicit solvers

As already pointed out, in a tokamak, the plasma presents several different space and time scales. It is not possible in practice to solve the initial Vlasov-Maxwell model. It is first necessary to establish asymptotic models by letting some parameters (such as the Larmor frequency or the speed of light) tend to infinity. This is the case for the electromagnetic solver and this requires implementing implicit time solvers in order to efficiently capture the stationary state, the solution of the magnetic induction equation or the Poisson equation.

VIRTUAL PLANTS Project-Team

3. Research Program

3.1. Analysis of structures resulting from meristem activity

To analyze plant growth and structure, we focus mainly on methods for analyzing sequences and tree-structured data. Theses methods range from algorithms for computing distance between sequences or tree-structured data to statistical models.

- *Combinatorial approaches*: plant structures exhibit complex branching organizations of their organs like internodes, leaves, shoots, axes, branches, etc. These structures can be analyzed with combinatorial methods in order to compare them or to reveal particular types of organization. We investigate a family of techniques to quantify distances between branching systems based on non-linear structural alignment (similar to edit-operation methods used for sequence comparison). Based on these techniques, we study the notion of (topology-based) self-similarity of branching structures in order to define a notion of degree of redundancy for any tree structure and to quantify in this way botanical notions, such as the physiological states of a meristem, fundamental to the description of plant morphogenesis.
- *Statistical modeling*: We investigate different categories of statistical models corresponding to different types of structures.
  - Longitudinal data corresponding to plant growth follow up: the statistical models of interest are equilibrium renewal processes and generalized linear mixed models for longitudinal count data.
  - Repeated patterns within sequences or trees: the statistical models of interest are mainly (hidden) variable-order Markov chains. Hidden variable-order Markov chains were in particular applied to characterize permutation patterns in phyllotaxis and the alternation between flowering and vegetative growth units along sympodial tree axes.
  - Homogeneous zones (or change points) within sequences or trees: most of the statistical models of interest are hidden Markovian models (hidden semi-Markov chains, semi-Markov switching linear mixed models and semi-Markov switching generalized linear models for sequences and different families of hidden Markov tree models). A complementary approach consists in applying multiple change-point models. The branching structure of a parent shoot is often organized as a succession of branching zones while the succession of shoot at the more macroscopic scale exhibit roughly stationary phases separated by marked change points.

  We investigate both estimation methods and diagnostic tools for these different categories of models. In particular we focus on diagnostic tools for latent structure models (e.g. hidden Markovian models or multiple change-point models) that consist in exploring the latent structure space.
- *A new generation of morphogenesis models*: Designing morphogenesis models of the plant development at the macroscopic scales is a challenging problem. As opposed to modeling approaches that attempt to describe plant development on the basis of the integration of purely mechanistic models of various plant functions, we intend to design models that tightly couple mechanistic and empirical sub-models that are elaborated in our plant architecture analysis approach. Empirical models are used as a powerful complementary source of knowledge in places where knowledge about mechanistic processes is lacking or weak. We chose to implement such integrated models in a programming language dedicated to dynamical systems with dynamical structure $(DS)^2$, such as L-systems or MGS. This type of language plays the role of an integration framework for sub-models of heterogeneous nature.

3.2. Meristem functioning and development

In this second scientific axis, we develop models of meristem growth at tissue level in order to integrate various sources of knowledge and to analyze their dynamic and complex spatial interaction. To carry out this integration, we need to develop a complete methodological approach containing:

- algorithms for the automatized segmentation in 3D, and cell lineage tracking throughout time, for images coming from confocal microscopy,
- design of high-level routines and user interfaces to distribute these image analysis tools to the scientific community,
- tools for structural and statistical analysis of 3D meristem structure (spatial statistics, multiscale geometric and topological analysis),
- physical models of cells interactions based on spring-mass systems or on tensorial mechanics at the level of cells,
- models of biochemical networks of hormonal and gene driven regulation, at the cellular and tissue level, using continuous and discrete formalisms,
- and models of cell development taking into account the effects of growth and cell divisions on the two previous classes of models.

VISAGES Project-Team

3. Research Program

3.1. Research Program

The scientific foundations of our team concern the development of new processing algorithms in the field of medical image computing : image fusion (registration and visualization), image segmentation and analysis, management of image related information. Since this is a very large domain, which can endorse numerous types of application; for seek of efficiency, the purpose of our methodological work primarily focuses on clinical aspects and for the most part on head and neck related diseases. In addition, we emphasize our research efforts on the neuroimaging domain. Concerning the scientific foundations, we have pushed our research efforts:

- In the field of image fusion and image registration (rigid and deformable transformations) with a special emphasis on new challenging registration issues, especially when statistical approaches based on joint histogram cannot be used or when the registration stage has to cope with loss or appearance of material (like in surgery or in tumor imaging for instance).
- In the field of image analysis and statistical modeling with a new focus on image feature and group analysis problems. A special attention was also to develop advanced frameworks for the construction of atlases and for automatic and supervised labeling of brain structures.
- In the field of image segmentation and structure recognition, with a special emphasis on the difficult problems of *i*) image restoration for new imaging sequences (new Magnetic Resonance Imaging protocols, 3D ultrasound sequences...), and *ii*) structure segmentation and labelling based on shape, multimodal and statistical information.
- Following the Neurobase national project where we had a leading role, we wanted to enhance the development of distributed and heterogeneous medical image processing systems.

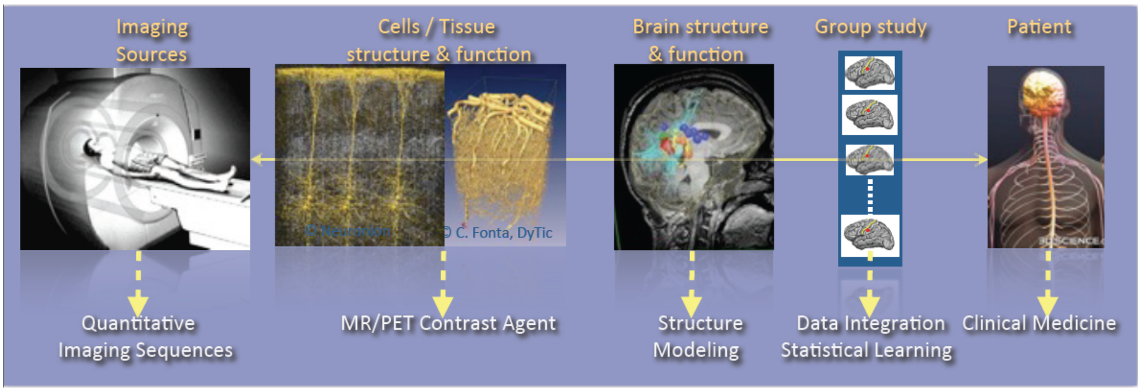

Figure 1. The major overall scientific foundation of the team concerns the integration of data from the Imaging source to the patient at different scales: from the cellular or molecular level describing the structure and function, to the functional and structural level of brain structures and regions, to the population level for the modelling of group patterns and the learning of group or individual imaging markers.

As shown in Fig. 1 , research activities of the VISAGES U746 team are tightly coupling observations and models through integration of clinical and multi-scale data, phenotypes (cellular, molecular or structural patterns). We work on personalized models of central nervous system organs and pathologies, and intend to confront these models to clinical investigation studies for quantitative diagnosis, prevention of diseases, therapy planning and validation. These approaches are developed in a translational framework where the data integration process to build the models inherits from specific clinical studies, and where the models are assessed on prospective clinical trials for diagnosis and therapy planning. All of this research activity is conducted in tight links with the Neurinfo imaging platform environments and the engineering staff of the platform. In this context, some of our major challenges in this domain concern:

- The elaboration of new descriptors to study the brain structure and function (e.g. variation of brain perfusion with and without contrast agent, evolution in shape and size of an anatomical structure in relation with normal, pathological or functional patterns, computation of asymmetries from shapes and volumes).
- The integration of additional spatio-temporal imaging sequences covering a larger range of observation, from the molecular level to the organ through the cell (Arterial Spin Labeling, diffusion MRI, MR relaxometry, MR cell labeling imaging, PET molecular imaging, . . .). This includes the elaboration of new image descriptors coming from spatio-temporal quantitative or contrast-enhanced MRI.
- The creation of computational models through data fusion of molecular, cellular, structural and functional image descriptors from group studies of normal and/or pathological subjects.
- The evaluation of these models on acute pathologies especially for the study of degenerative, psychiatric or developmental brain diseases (e.g. Multiple Sclerosis, Epilepsy, Parkinson, Dementia, Strokes, Depression, Schizophrenia, . . .) in a translational framework.

In terms of methodological developments, we are particularly working on statistical methods for multidimensional image analysis, and feature selection and discovery, which includes:

- The development of specific shape and appearance models, construction of atlases better adapted to a patient or a group of patients in order to better characterize the pathology;
- The development of advanced segmentation and modeling methods dealing with longitudinal and multidimensional data (vector or tensor fields), especially with the integration of new prior models to control the integration of multiscale data and aggregation of models;
- The development of new models and probabilistic methods to create water diffusion maps from MRI;
- The integration of machine learning procedures for classification and labeling of multidimensional features (from scalar to tensor fields and/or geometric features): pattern and rule inference and knowledge extraction are key techniques to help in the elaboration of knowledge in the complex domains we address;
- The development of new dimensionality reduction techniques for problems with massive data, which includes dictionary learning for sparse model discovery. Efficient techniques have still to be developed to properly extract from a raw mass of images derived data that are easier to analyze.

XPOP Team

3. Research Program

3.1. Scientific positioning

"Interfaces" is the defining characteristic of XPOP:

The interface between statistics, probability and numerical methods. Mathematical modelling of complex biological phenomena require to combine numerical, stochastic and statistical approaches. The CMAP is therefore the right place to be for positioning the team at the interface between several mathematical disciplines.

The interface between mathematics and the life sciences. The goal of XPOP is to bring the right answers to the right questions. These answers are mathematical tools (statistics, numerical methods, etc.), whereas the questions come from the life sciences (pharmacology, medicine, biology, etc.). This is why the point of XPOP is not to take part in mathematical projects only, but also pluridisciplinary ones.

The interface between mathematics and software development. The development of new methods is the main activity of XPOP. However, new methods are only useful if they end up being implemented in a software tool. A strong partnership with Lixoft (the spin-off company who continue developing MONOLIX) is indispensable to maintaining this positioning.

3.2. The mixed-effects models

Mixed-effects models are statistical models with both fixed effects and random effects. They are well-adapted to situations where repeated measurements are made on the same individual/statistical unit.

Consider first a single subject i of the population. Let $y_i = (y_{ij}, 1 \leq j \leq n_i)$ be the vector of observations for this subject. The model that describes the observations y_i is assumed to be a parametric probabilistic model: let $p_Y(y_i; \psi_i)$ be the probability distribution of y_i, where ψ_i is a vector of parameters.

In a population framework, the vector of parameters ψ_i is assumed to be drawn from a population distribution $p_\Psi(\psi_i; \theta)$ where θ is a vector of population parameters.

Then, the probabilistic model is the joint probability distribution

$$p(y_i, \psi_i; \theta) = p_Y(y_i|\psi_i)p_\Psi(\psi_i; \theta) \tag{89}$$

To define a model thus consists in defining precisely these two terms.

In most applications, the observed data y_i are continuous longitudinal data. We then assume the following representation for y_i:

$$y_{ij} = f(t_{ij}, \psi_i) + g(t_{ij}, \psi_i)\varepsilon_{ij} \quad , \quad 1 \leq i \leq N \quad , \quad 1 \leq j \leq n_i. \tag{90}$$

Here, y_{ij} is the observation obtained from subject i at time t_{ij}. The residual errors (ε_{ij}) are assumed to be standardized random variables (mean zero and variance 1). The residual error model is represented by function g in model (2).

Function f is usually the solution to a system of ordinary differential equations (pharmacokinetic/pharmacodynamic models, etc.) or a system of partial differential equations (tumor growth, respiratory system, etc.). This component is a fundamental component of the model since it defines the prediction of the observed kinetics for a given set of parameters.

The vector of individual parameters ψ_i is usually function of a vector of population parameters $\psi_{\rm pop}$, a vector of random effects $\eta_i \sim \mathcal{N}(0,\Omega)$, a vector of individual covariates c_i (weight, age, gender, ...) and some fixed effects β.

The joint model of y and ψ depends then on a vector of parameters $\theta = (\psi_{\rm pop}, \beta, \Omega)$.

3.3. Computational Statistical Methods

Central to modern statistics is the use of probabilistic models. To relate these models to data requires the ability to calculate the probability of the observed data: the likelihood function, which is central to most statistical methods and provides a principled framework to handle uncertainty.

The emergence of computational statistics as a collection of powerful and general methodologies for carrying out likelihood-based inference made complex models with non-standard data accessible to likelihood, including hierarchical models, models with intricate latent structure, and missing data.

In particular, algorithms previously developed by POPIX for mixed effects models, and today implemented in several software tools (especially MONOLIX) are part of these methods:

- the adaptive Metropolis-Hastings algorithm allows one to sample from the conditional distribution of the individual parameters $p(\psi_i|y_i;c_i,\theta)$,
- the SAEM algorithm is used to maximize the observed likelihood $\mathcal{L}(\theta;y) = p(y;\theta)$,
- Importance Sampling Monte Carlo simulations provide an accurate estimation of the observed log-likelihood $\log(\mathcal{L}(\theta;y))$.

Computational statistics is an area which remains extremely active today. Recently, one can notice that the incentive for further improvements and innovation comes mainly from three broad directions: the high dimensional challenge, the quest for adaptive procedures that can eliminate the cumbersome process of tuning "by hand" the settings of the algorithms and the need for flexible theoretical support, arguably required by all recent developments as well as many of the traditional MCMC algorithms that are widely used in practice.

Working in these three directions is a clear objective for XPOP.

3.4. Markov Chain Monte Carlo algorithms

While these Monte Carlo algorithms have turned into standard tools over the past decade, they still face difficulties in handling less regular problems such as those involved in deriving inference for high-dimensional models. One of the main problems encountered when using MCMC in this challenging settings is that it is difficult to design a Markov chain that efficiently samples the state space of interest.

The Metropolis-adjusted Langevin algorithm (MALA) is a Markov chain Monte Carlo (MCMC) method for obtaining random samples from a probability distribution for which direct sampling is difficult. As the name suggests, MALA uses a combination of two mechanisms to generate the states of a random walk that has the target probability distribution as an invariant measure:

1. new states are proposed using Langevin dynamics, which use evaluations of the gradient of the target probability density function;
2. these proposals are accepted or rejected using the Metropolis-Hastings algorithm, which uses evaluations of the target probability density (but not its gradient).

Informally, the Langevin dynamics drives the random walk towards regions of high probability in the manner of a gradient flow, while the Metropolis-Hastings accept/reject mechanism improves the mixing and convergence properties of this random walk.

Several extensions of MALA have been proposed recently by several authors, including fMALA (fast MALA), AMALA (anisotropic MALA), MMALA (manifold MALA), position-dependent MALA (PMALA), ...

MALA and these extensions have demonstrated to represent very efficient alternative for sampling from high dimensional distributions. We therefore need to adapt these methods to general mixed effects models.

3.5. Parameter estimation

The Stochastic Approximation Expectation Maximization (SAEM) algorithm has shown to be extremely efficient for maximum likelihood estimation in incomplete data models, and particularly in mixed effects models for estimating the population parameters. However, there are several practical situations for which extensions of SAEM are still needed:

High dimensional model: a complex physiological model may have a large number of parameters (in the order of 100). Then several problems arise:

- when most of these parameters are associated with random effects, the MCMC algorithm should be able to sample, for each of the N individuals, parameters from a high dimensional distribution. Efficient MCMC methods for high dimensions are then required.
- Practical identifiability of the model is not ensured with a limited amount of data. In other words, we cannot expect to be able to properly estimate all the parameters of the model, including the fixed effects and the variance-covariance matrix of the random effects. Then, some random effects should be removed, assuming that some parameters do not vary in the population. It may also be necessary to fix the value of some parameters (using values from the literature for instance). The strategy to decide which parameters should be fixed and which random effects should be removed remains totally empirical. XPOP aims to develop a procedure that will help the modeller to take such decisions.

Large number of covariates: the covariate model aims to explain part of the inter-patient variability of some parameters. Classical methods for covariate model building are based on comparisons with respect to some criteria, usually derived from the likelihood (AIC, BIC), or some statistical test (Wald test, LRT, etc.). In other words, the modelling procedure requires two steps: first, all possible models are fitted using some estimation procedure (e.g. the SAEM algorithm) and the likelihood of each model is computed using a numerical integration procedure (e.g. Monte Carlo Importance Sampling); then, a model selection procedure chooses the "best" covariate model. Such a strategy is only possible with a reduced number of covariates, i.e., with a "small" number of models to fit and compare.

As an alternative, we are thinking about a Bayesian approach which consists of estimating simultaneously the covariate model and the parameters of the model in a single run. An (informative or uninformative) prior is defined for each model by defining a prior probability for each covariate to be included in the model. In other words, we extend the probabilistic model by introducing binary variables that indicate the presence or absence of each covariate in the model. Then, the model selection procedure consists of estimating and maximizing the conditional distribution of this sequence of binary variables. Furthermore, a probability can be associated to any of the possible covariate models.

This conditional distribution can be estimated using an MCMC procedure combined with the SAEM algorithm for estimating the population parameters of the model. In practice, such an approach can only deal with a limited number of covariates since the dimension of the probability space to explore increases exponentially with the number of covariates. Consequently, we would like to have methods able to find a small number of variables (from a large starting set) that influence certain parameters in populations of individuals. That means that, instead of estimating the conditional distribution of all the covariate models as described above, the algorithm should focus on the most likely ones.

Fixed parameters: it is quite frequent that some individual parameters of the model have no random component and are purely fixed effects. Then, the model may not belong to the exponential family anymore and the original version of SAEM cannot be used as it is. Several extensions exist:

- introduce random effects with decreasing variances for these parameters,
- introduce a prior distribution for these fixed effects,
- apply the stochastic approximation directly on the sequence of estimated parameters, instead of the sufficient statistics of the model.

None of these methods always work correctly. Furthermore, what are the pros and cons of these methods is not clear at all. Then, developing a robust methodology for such model is necessary.

Convergence toward the global maximum of the likelihood: convergence of SAEM can strongly depend on thie initial guess when the observed likelihood has several local maxima. A kind of simulated annealing version of SAEM was previously developed and implemented in MONOLIX. The method works quite well in most situations but there is no theoretical justification and choosing the settings of this algorithm (i.e. how the temperature decreases during the iterations) remains empirical. A precise analysis of the algorithm could be very useful to better understand why it "works" in practice and how to optimize it.

Convergence diagnostic: Convergence of SAEM was theoretically demonstrated under very general hypothesis. Such result is important but of little interest in practice at the time to use SAEM in a finite amount of time, i.e. in a finite number of iterations. Some qualitative and quantitative criteria should be defined in order to both optimize the settings of the algorithm, detect a poor convergence of SAEM and evaluate the quality of the results in order to avoid using them unwisely.

3.6. Model building

Defining an optimal strategy for model building is far from easy because a model is the assembled product of numerous components that need to been evaluated and perhaps improved: the structural model, residual error model, covariate model, covariance model, etc.

How to proceed so as to obtain the best possible combination of these components? There is no magic recipe but an effort will be made to provide some qualitative and quantitative criteria in order to help the modeller for building his model.

The strategy to take will mainly depend on the time we can dedicate to building the model and the time required for running it. For relatively simple models for which parameter estimation is fast, it is possible to fit many models and compare them. This can also be done if we have powerful computing facilities available (e.g., a cluster) allowing large numbers of simultaneous runs.

However, if we are working on a standard laptop or desktop computer, model building is a sequential process in which a new model is tested at each step. If the model is complex and requires significant computation time (e.g., when involving systems of ODEs), we are constrained to limit the number of models we can test in a reasonable time period. In this context, it also becomes important to carefully choose the tasks to run at each step.

3.7. Model evaluation

Diagnostic tools are recognized as an essential method for model assessment in the process of model building. Indeed, the modeler needs to confront "his" model with the experimental data before concluding that this model is able to reproduce the data and before using it for any purpose, such as prediction or simulation for instance.

The objective of a diagnostic tool is twofold: first we want to check if the assumptions made on the model are valid or not ; then, if some assumptions are rejected, we want to get some guidance on how to improve the model.

As is the usual case in statistics, it is not because this "final" model has not been rejected that it is necessarily the "true" one. All that we can say is that the experimental data does not allow us to reject it. It is merely one of perhaps many models that cannot be rejected.

Model diagnostic tools are for the most part graphical, i.e., visual; we "see" when something is not right between a chosen model and the data it is hypothesized to describe. These diagnostic plots are usually based on the empirical Bayes estimates (EBEs) of the individual parameters and EBEs of the random effects: scatterplots of individual parameters versus covariates to detect some possible relationship, scatterplots of pairs of random effects to detect some possible correlation between random effects, plot of the empirical distribution of the random effects (boxplot, histogram,...) to check if they are normally distributed, ...

The use of EBEs for diagnostic plots and statistical tests is efficient with rich data, i.e. when a significant amount of information is available in the data for recovering accurately all the individual parameters. On the contrary, tests and plots can be misleading when the estimates of the individual parameters are greatly shrunk.

We propose to develop new approaches for diagnosing mixed effects models in a general context and derive formal and unbiased statistical tests for testing separately each feature of the model.

3.8. Missing data

The ability to easily collect and gather a large amount of data from different sources can be seen as an opportunity to better understand many processes. It has already led to breakthroughs in several application areas. However, due to the wide heterogeneity of measurements and objectives, these large databases often exhibit an extraordinary high number of missing values. Hence, in addition to scientific questions, such data also present some important methodological and technical challenges for data analyst.

Missing values occur for a variety of reasons: machines that fail, survey participants who do not answer certain questions, destroyed or lost data, dead animals, damaged plants, etc. Missing values are problematic since most statistical methods can not be applied directly on a incomplete data. Many progress have been made to properly handle missing values. However, there are still many challenges that need to be addressed in the future, that are crucial for the users.

- State of arts methods often consider the case of continuous or categorical data whereas real data are very often mixed. The idea is to develop a multiple imputation method based on a specific principal component analysis (PCA) for mixed data. Indeed, PCA has been used with success to predict (impute) the missing values. A very appealing property is the ability of the method to handle very large matrices with large amount of missing entries.
- The asymptotic regime underlying modern data is not any more to consider that the sample size increases but that both number of observations and number of variables are very large. In practice first experiments showed that the coverage properties of confidence areas based on the classical methods to estimate variance with missing values varied widely. The asymptotic method and the bootstrap do well in low-noise setting, but can fail when the noise level gets high or when the number of variables is much greater than the number of rows. On the other hand, the jackknife has good coverage properties for large noisy examples but requires a minimum number of variables to be stable enough.
- Inference with missing values is usually performed under the assumption of "Missing at Random" (MAR) values which means that the probability that a value is missing may depend on the observed data but does not depend on the missing value itself. In real data and in particular in data coming from clinical studies, both "Missing Non at Random" (MNAR) and MAR values occur. Taking into account in a proper way both types of missing values is extremely challenging but is worth investigating since the applications are extremely broad.

It is important to stress that missing data models are part of the general incomplete data models addressed by XPOP. Indeed, models with latent variables (i.e. non observed variables such as random effects in a mixed effects model), models with censored data (e.g. data below some limit of quantification) or models with dropout mechanism (e.g. when a subject in a clinical trial fails to continue in the study) can be seen as missing data models.

ALPINES Project-Team

3. Research Program

3.1. Overview

The research described here is directly relevant to several steps of the numerical simulation chain. Given a numerical simulation that was expressed as a set of differential equations, our research focuses on mesh generation methods for parallel computation, novel numerical algorithms for linear algebra, as well as algorithms and tools for their efficient and scalable implementation on high performance computers. The validation and the exploitation of the results is performed with collaborators from applications and is based on the usage of existing tools. In summary, the topics studied in our group are the following:

- Numerical methods and algorithms
  - Mesh generation for parallel computation
  - Solvers for numerical linear algebra
  - Computational kernels for numerical linear algebra
- Validation on numerical simulations

3.2. Domain specific language - parallel FreeFem++

In the engineering, researchers, and teachers communities, there is a strong demand for simulation frameworks that are simple to install and use, efficient, sustainable, and that solve efficiently and accurately complex problems for which there are no dedicated tools or codes available. In our group we develop FreeFem++ (see http://www.freefem.org/ff++), a user dedicated language for solving PDEs. The goal of FreeFem++ is not to be a substitute for complex numerical codes, but rather to provide an efficient and relatively generic tool for:

- getting a quick answer to a specific problem,
- prototyping the resolution of a new complex problem.

The current users of FreeFem++ are mathematicians, engineers, university professors, and students. In general for these users the installation of public libraries as MPI, MUMPS, Ipopt, Blas, lapack, OpenGL, fftw, scotch, is a very difficult problem. For this reason, the authors of FreeFem++ have created a user friendly language, and over years have enriched its capabilities and provided tools for compiling FreeFem++ such that the users do not need to have special knowledge of computer science. This leads to an important work on porting the software on different emerging architectures.

Today, the main components of parallel FreeFem++ are:

1. definition of a coarse grid,
2. splitting of the coarse grid,
3. mesh generation of all subdomains of the coarse grid, and construction of parallel datat structures for vectors and sparse matrices from the mesh of the subdomain,
4. call to a linear solver,
5. analysis of the result.

All these components are parallel, except for point (5) which is not in the focus of our research. However for the moment, the parallel mesh generation algorithm is very simple and not sufficient, for example it addresses only polygonal geometries. Having a better parallel mesh generation algorithm is one of the goals of our project. In addition, in the current version of FreeFem++, the parallelism is not hidden from the user, it is done through direct calls to MPI. Our goal is also to hide all the MPI calls in the specific language part of FreeFem++.

3.3. Solvers for numerical linear algebra

Iterative methods are widely used in industrial applications, and preconditioning is the most important research subject here. Our research considers domain decomposition methods and iterative methods and its goal is to develop solvers that are suitable for parallelism and that exploit the fact that the matrices are arising from the discretization of a system of PDEs on unstructured grids.

One of the main challenges that we address is the lack of robustness and scalability of existing methods as incomplete LU factorizations or Schwarz-based approaches, for which the number of iterations increases significantly with the problem size or with the number of processors. This is often due to the presence of several low frequency modes that hinder the convergence of the iterative method. To address this problem, we study direction preserving solvers in the context of multilevel domain decomposition methods with adaptive coarse spaces and multilevel incomplete decompositions. A judicious choice for the directions to be preserved through filtering or low rank approximations allows us to alleviate the effect of low frequency modes on the convergence.

We also focus on developing boundary integral equation methods that would be adapted to the simulation of wave propagation in complex physical situations, and that would lend themselves to the use of parallel architectures, which includes devising adapted domain decomposition approaches. The final objective is to bring the state of the art on boundary integral equations closer to contemporary industrial needs.

3.4. Computational kernels for numerical linear algebra

The design of new numerical methods that are robust and that have well proven convergence properties is one of the challenges addressed in Alpines. Another important challenge is the design of parallel algorithms for the novel numerical methods and the underlying building blocks from numerical linear algebra. The goal is to enable their efficient execution on a diverse set of node architectures and their scaling to emerging high-performance clusters with an increasing number of nodes.

Increased communication cost is one of the main challenges in high performance computing that we address in our research by investigating algorithms that minimize communication, as communication avoiding algorithms. We propose to integrate the minimization of communication into the algorithmic design of numerical linear algebra problems. This is different from previous approaches where the communication problem was addressed as a scheduling or as a tuning problem. The communication avoiding algorithmic design is an aproach originally developed in our group since 2007 (initially in collaboration with researchers from UC Berkeley and CU Denver). While at mid term we focus on reducing communication in numerical linear algebra, at long term we aim at considering the communication problem one level higher, during the parallel mesh generation tool described earlier.

ASAP Project-Team

3. Research Program

3.1. Theory of distributed systems

Finding models for distributed computations prone to asynchrony and failures has received a lot of attention. A lot of research in this domain focuses on what can be computed in such models, and, when a problem can be solved, what are its best solutions in terms of relevant cost criteria. An important part of that research is focused on distributed computability: what can be computed when failure detectors are combined with conditions on process input values for example. Another part is devoted to model equivalence. What can be computed with a given class of failure detectors? Which synchronization primitives is a given failure class equivalent to? These are among the main topics addressed in the leading distributed computing community. A second fundamental issue related to distributed models is the definition of appropriate models suited to dynamic systems. Up to now, the researchers in that area consider that nodes can enter and leave the system, but do not provide a simple characterization, based on properties of computation instead of description of possible behaviors [58], [51], [53]. This shows that finding dynamic distributed computing models is today a "Holy Grail", whose discovery would allow a better understanding of the essential nature of dynamic systems.

3.2. Peer-to-peer overlay networks

A standard distributed system today is related to thousands or even millions of computing entities scattered all over the world and dealing with a huge amount of data. This major shift in scalability requirements has lead to the emergence of novel computing paradigms. In particular, the peer-to-peer communication paradigm imposed itself as the prevalent model to cope with the requirements of large scale distributed systems. Peer-to-peer systems rely on a symmetric communication model where peers are potentially both clients and servers. They are fully decentralized, thus avoiding the bottleneck imposed by the presence of servers in traditional systems. They are highly resilient to peers arrivals and departures. Finally, individual peer behavior is based on a local knowledge of the system and yet the system converges toward global properties.

A peer-to-peer overlay network logically connects peers on top of IP. Two main classes of such overlays dominate, structured and unstructured. The differences relate to the choice of the neighbors in the overlay, and the presence of an underlying naming structure. Overlay networks represent the main approach to build large-scale distributed systems that we retained. An overlay network forms a logical structure connecting participating entities on top of the physical network, be it IP or a wireless network. Such an overlay might form a structured overlay network [59], [60], [61] following a specific topology or an unstructured network [56], [62] where participating entities are connected in a random or pseudo-random fashion. In between, lie weakly structured peer-to-peer overlays where nodes are linked depending on a proximity measure providing more flexibility than structured overlays and better performance than fully unstructured ones. Proximity-aware overlays connect participating entities so that they are connected to close neighbors according to a given proximity metric reflecting some degree of affinity (computation, interest, etc.) between peers. We extensively use this approach to provide algorithmic foundations of large-scale dynamic systems.

3.3. Epidemic protocols

Epidemic algorithms, also called gossip-based algorithms [55], [54], constitute a fundamental topic in our research. In the context of distributed systems, epidemic protocols are mainly used to create overlay networks and to ensure a reliable information dissemination in a large-scale distributed system. The principle underlying technique, in analogy with the spread of a rumor among humans via gossiping, is that participating entities continuously exchange information about the system in order to spread it gradually and reliably. Epidemic algorithms have proved efficient to build and maintain large-scale distributed systems in the context of many applications such as broadcasting [54], monitoring, resource management, search, and more generally in building unstructured peer-to-peer networks.

3.4. Malicious process behaviors

When assuming that processes fail by simply crashing, bounds on resiliency (maximum number of processes that may crash, number of exchanged messages, number of communication steps, etc.) are known both for synchronous and augmented asynchronous systems (recall that in purely asynchronous systems some problems are impossible to solve). If processes can exhibit malicious behaviors, these bounds are seldom the same. Sometimes, it is even necessary to change the specification of the problem. For example, the consensus problem for correct processes does not make sense if some processes can exhibit a Byzantine behavior and thus propose an arbitrary value. In this case, the validity property of consensus, which is normally "a decided value is a proposed value", must be changed to "if all correct processes propose the same value then only this value can be decided." Moreover, the resilience bound of less than half of faulty processes is at least lowered to "less than a third of Byzantine processes." These are some of the aspects that underlie our studies in the context of the classical model of distributed systems, in peer-to-peer systems and in sensor networks.

3.5. Online social networks and recommender systems

Social Networks have rapidly become a fundamental component of today's distributed applications. Web 2.0 applications have dramatically changed the way users interact with the Internet and with each other. The number of users of websites like Flickr, Delicious, Facebook, or MySpace is constantly growing, leading to significant technical challenges. On the one hand, these websites are called to handle enormous amounts of data. On the other hand, news continue to report the emergence of privacy threats to the personal data of social-network users. Our research aims to exploit our expertise in distributed systems to lead to a new generation of scalable, privacy-preserving, social applications.

We also investigate approaches to build implicit social networks, connecting users sharing similar interests. At the heart of the building of such similarity graphs lie k-nearest neighbor (KNN) algorithms. Our research in this area is to design and implement efficient KNN algorithms able to cope with a huge volume of data as well as a high level of dynamism. We investigate the use of such similarity graphs to build highly scalable infrastructures for recommendation systems.

3. Research Program

3.1. Overview

Since we mainly work on new concepts for the language-based definition and implementation of complex software systems, we first briefly introduce some basic notions and problems of software components (understood in a broad sense, that is, including modules, objects, architecture description languages and services), aspects, and domain-specific languages. We conclude by presenting the main issues related to distribution and concurrency, in particular related to capacity planning issues that are relevant to our work.

3.2. Software Composition

Modules and services. The idea that building *software components*, i.e., composable prefabricated and parameterized software parts, was key to create an effective software industry was realized very early [72]. At that time, the scope of a component was limited to a single procedure. In the seventies, the growing complexity of software made it necessary to consider a new level of structuring and programming and led to the notions of information hiding, *modules*, and module interconnection languages [79], [55]. Information hiding promotes a black-box model of program development whereby a module implementation, basically a collection of procedures, is strongly encapsulated behind an interface. This makes it possible to guarantee logical invariant *properties* of the data managed by the procedures and, more generally, makes *modular reasoning* possible.

In the context of today's Internet-based information society, components and modules have given rise to *software services* whose compositions are governed by explicit *orchestration or choreography* specifications that support notions of global properties of a service-oriented architecture. These horizontal compositions have, however, to be frequently adapted dynamically. Dynamic adaptations, in particular in the context of software evolution processes, often conflict with a black-box composition model either because of the need for invasive modifications, for instance, in order to optimize resource utilization or modifications to the vertical compositions implementing the high-level services.

Object-Oriented Programming. Classes and objects provide another kind of software component, which makes it necessary to distinguish between *component types* (classes) and *component instances* (objects). Indeed, unlike modules, objects can be created dynamically. Although it is also possible to talk about classes in terms of interfaces and implementations, the encapsulation provided by classes is not as strong as the one provided by modules. This is because, through the use of inheritance, object-oriented languages put the emphasis on *incremental programming* to the detriment of modular programming. This introduces a white-box model of software development and more flexibility is traded for safety as demonstrated by the *fragile base class* issue [75].

Architecture Description Languages. The advent of distributed applications made it necessary to consider more sophisticated connections between the various building blocks of a system. The *software architecture* [84] of a software system describes the system as a composition of *components* and *connectors*, where the connectors capture the *interaction protocols* between the components [43]. It also describes the rationale behind such a given architecture, linking the properties required from the system to its implementation. *Architecture Description Languages* (ADLs) are languages that support architecture-based development [73]. A number of these languages make it possible to generate executable systems from architectural descriptions, provided implementations for the primitive components are available. However, guaranteeing that the implementation conforms to the architecture is an issue.

Protocols. Today, protocols constitute a frequently used means to precisely define, implement, and analyze contracts, notably concerning communication and security properties, between two or more hardware or software entities. They have been used to define interactions between communication layers, security properties of distributed communications, interactions between objects and components, and business processes.

Object interactions [77], component interactions [90], [81] and service orchestrations [56] are most frequently expressed in terms of *regular interaction protocols* that enable basic properties, such as compatibility, substitutability, and deadlocks between components to be defined in terms of basic operations and closure properties of finite-state automata. Furthermore, such properties may be analyzed automatically using, e.g., model checking techniques [53], [62].

However, the limited expressive power of regular languages has led to a number of approaches using more expressive *non-regular* interaction protocols that often provide distribution-specific abstractions, e.g., session types [66], or context-free or turing-complete expressiveness [82], [50]. While these protocol types allow conformance between components to be defined (e.g., using unbounded counters), property verification can only be performed manually or semi-automatically.

3.3. Programming languages for advanced modularization

The main driving force for the structuring means, such as components and modules, is the quest for clean *separation of concerns* [57] on the architectural and programming levels. It has, however, early been noted that concern separation in the presence of crosscutting functionalities requires specific language and implementation level support. Techniques of so-called *computational reflection*, for instance, Smith's 3-Lisp or Kiczales's CLOS meta-object protocol [85], [69] as well as metaprogramming techniques have been developed to cope with this problem but proven unwieldy to use and not amenable to formalization and property analysis due to their generality. Methods and techniques from two fields have been particularly useful in addressing such advanced modularization problems: Aspect-Oriented Software Development as the field concerned with the systematic handling of modularization issues and domain-specific languages that provide declarative and efficient means for the definition of crosscutting functionalities.

Aspect-Oriented Software Development [68], [41] has emerged over the previous decade as the domain of systematic exploration of crosscutting concerns and corresponding support throughout the software development process. The corresponding research efforts have resulted, in particular, in the recognition of *crosscutting* as a fundamental problem of virtually any large-scale application, and the definition and implementation of a large number of aspect-oriented models and languages.

However, most current aspect-oriented models, notably AspectJ [67], rely on pointcuts and advice defined in terms of individual execution events. These models are subject to serious limitations concerning the modularization of crosscutting functionalities in distributed applications, the integration of aspects with other modularization mechanisms such as components, and the provision of correctness guarantees of the resulting AO applications. They do, in particular, only permit the manipulation of distributed applications on a per-host basis, that is, without direct expression of coordination properties relating different distributed entities [86]. Similarly, current approaches for the integration of aspects and (distributed) components do not directly express interaction properties between sets of components but rather seemingly unrelated modifications to individual components [54]. Finally, current formalizations of such aspect models are formulated in terms of low-level semantic abstractions (see, e.g., Wand's et al semantics for AspectJ [89]) and provide only limited support for the analysis of fundamental aspect properties.

Different approaches have been put forward to tackle these problems, in particular, in the context of so-called *stateful* or *history-based aspect languages* [58], [59], which provide pointcut and advice languages that directly express rich relationships between execution events. Such languages have been proposed to directly express coordination and synchronization issues of distributed and concurrent applications [78], [48], [61], provide more concise formal semantics for aspects and enable analysis of their properties [44], [60], [58], [42]. Furthermore, first approaches for the definition of *aspects over protocols* have been proposed, as well as over regular structures [58] and non-regular ones [88], [76], which are helpful for the modular definition and verification of protocols over crosscutting functionalities.

They represent, however, only first results and many important questions concerning these fundamental issues remain open, in particular, concerning the semantics foundations of AOP and the analysis and enforcement of correctness properties governing its, potentially highly invasive, modifications.

Domain-specific languages (DSLs) represent domain knowledge in terms of suitable basic language constructs and their compositions at the language level. By trading generality for abstraction, they enable complex relationships among domain concepts to be expressed concisely and their properties to be expressed and formally analyzed. DSLs have been applied to a large number of domains; they have been particularly popular in the domain of software generation and maintenance [74], [92].

Many modularization techniques and tasks can be naturally expressed by DSLs that are either specialized with respect to the type of modularization constructs, such as a specific brand of software component, or to the compositions that are admissible in the context of an application domain that is targeted by a modular implementation. Moreover, software development and evolution processes can frequently be expressed by transformations between applications implemented using different DSLs that represent an implementation at different abstraction levels or different parts of one application.

Functionalities that crosscut a component-based application, however, complicate such a DSL-based transformational software development process. Since such functionalities belong to another domain than that captured by the components, different DSLs should be composed. Such compositions (including their syntactic expression, semantics and property analysis) have only very partially been explored until now. Furthermore, restricted composition languages and many aspect languages that only match execution events of a specific domain (e.g., specific file accesses in the case of security functionality) and trigger only domain-specific actions clearly are quite similar to DSLs but remain to be explored.

3.4. Distribution and Concurrency

While ASCOLA does not investigate distribution and concurrency as research domains per se (but rather from a software engineering and modularization viewpoint), there are several specific problems and corresponding approaches in these domains that are directly related to its core interests that include the structuring and modularization of large-scale distributed infrastructures and applications. These problems include crosscutting functionalities of distributed and concurrent systems, support for the evolution of distributed software systems, and correctness guarantees for the resulting software systems.

Underlying our interest in these domains is the well-known observation that large-scale distributed applications are subject to *numerous crosscutting functionalities* (such as the transactional behavior in enterprise information systems, the implementation of security policies, and fault recovery strategies). These functionalities are typically partially encapsulated in distributed infrastructures and partially handled in an ad hoc manner by using infrastructure services at the application level. Support for a more principled approach to the development and evolution of distributed software systems in the presence of crosscutting functionalities has been investigated in the field of *open adaptable middleware* [49], [71]. Open middleware design exploits the concept of reflection to provide the desired level of configurability and openness. However, these approaches are subject to several fundamental problems. One important problem is their insufficient, framework-based support that only allows partial modularization of crosscutting functionalities.

There has been some *criticism* on the use of *AspectJ-like aspect models* (which middleware aspect models like that of JBoss AOP are an instance of) for the modularization of distribution and concurrency related concerns, in particular, for transaction concerns [70] and the modularization of the distribution concern itself [86]. Both criticisms are essentially grounded in AspectJ's inability to explicitly represent sophisticated relationships between execution events in a distributed system: such aspects therefore cannot capture the semantic relationships that are essential for the corresponding concerns. History-based aspects, as those proposed by the ASCOLA project-team provide a starting point that is not subject to this problem.

From a point of view of language design and implementation, aspect languages, as well as domain specific languages for distributed and concurrent environments share many characteristics with existing distributed languages: for instance, event monitoring is fundamental for pointcut matching, different synchronization strategies and strategies for code mobility [64] may be used in actions triggered by pointcuts. However, these relationships have only been explored to a small degree. Similarly, the formal semantics and formal properties of aspect languages have not been studied yet for the distributed case and only rudimentarily for the concurrent one [44], [61].

3.5. Security

Security properties and policies over complex service-oriented and standalone applications become ever more important in the context of asynchronous and decentralized communicating systems. Furthermore, they constitute prime examples of crosscutting functionalities that can only be modularized in highly insufficient ways with existing programming language and service models. Security properties and related properties, such as accountability properties, are therefore very frequently awkward to express and difficult to analyze and enforce (provided they can be made explicit in the first place).

Two main issues in this space are particularly problematic from a compositional point of view. First, information flow properties of programming languages, such as flow properties of Javascript [46], and service-based systems [52] are typically specially-tailored to specific properties, as well as difficult to express and analyze. Second, the enforcement of security properties and security policies, especially accountability-related properties [80], [87], is only supported using ad hoc means with rudimentary support for property verification.

The ASCOLA team has recently started to work on providing formal methods, language support and implementation techniques for the modular definition and implementation of information flow properties as well as policy enforcement in service-oriented systems as well as, mostly object-oriented, programming languages.

3.6. Green IT

With the emergence of the Future Internet and the dawn of new IT architecture and computation models such as cloud computing, the usage of data centers (DC) as well as their power consumption increase dramatically [51]. Besides the ecological impact [65], energy consumption is a predominant criterion for DC providers since it determines the daily cost of their infrastructure. As a consequence, power management becomes one of the main challenges for DC infrastructures and more generally for large-scale distributed systems.

To address this problem, we study two approaches: a workload-driven [47] and power-driven one [83]. As part of the workload-driven solution, we adapt the power consumption of the DC depending on the application workload, and evaluate whether this workload to be more reactive. We develop a distributed system from the system to the service-oriented level mainly based on hardware and virtualization capabilities that is managed in a user-transparent fashion. As part of the power-driven approach, we address energy consumption issues through a strong synergy inside the infrastructure software stack and more precisely between applications and resource management systems. This approach is characterized by adapting QoS properties aiming at the best trade-off between cost of energy (typically from the regular electric grid), its availability (for instance, from renewable energy), and service degradation caused, for instance, by application reconfigurations to jobs suspensions.

3.7. Capacity Planning for Large Scale Distributed System

Since the last decade, cloud computing has emerged as both a new economic model for software (provision) and as flexible tools for the management of computing capacity [45]. Nowadays, the major cloud features have become part of the mainstream (virtualization, storage and software image management) and the big market players offer effective cloud-based solutions for resource pooling. It is now possible to deploy virtual infrastructures that involve virtual machines (VMs), middleware, applications, and networks in such a simple manner that a new problem has emerged since 2010: VM sprawl (virtual machine proliferation) that consumes valuable computing, memory, storage and energy resources, thus menacing serious resource shortages. Scientific approaches that address VM sprawl are both based on classical administration techniques like the lifecycle management of a large number of VMs as well as the arbitration and the careful management of all resources consumed and provided by the hosting infrastructure (energy, power, computing, memory, network etc.) [63], [91].

The ASCOLA team investigates fundamental techniques for cloud computing and capacity planning, from infrastructures to the application level. Capacity planning is the process of planning for, analyzing, sizing, managing and optimizing capacity to satisfy demand in a timely manner and at a reasonable cost. Applied to distributed systems like clouds, a capacity planning solution must mainly provide the minimal set of resources necessary for the proper execution of the applications (i.e., to ensure SLA). The main challenges in this context are: scalability, fault tolerance and reactivity of the solution in a large-scale distributed system, the analysis and optimization of resources to minimize the cost (mainly costs related to the energy consumption of datacenters), as well as the profiling and adaptation of applications to ensure useful levels of quality of service (throughput, response time, availability etc.).

Our solutions are mainly based on virtualized infrastructures that we apply from the IaaS to the SaaS levels. We are mainly concerned by the management and the execution of the applications by harnessing virtualization capabilities, the investigation of alternative solutions that aim at optimizing the trade-off between performance and energy costs of both applications and cloud resources, as well as arbitration policies in the cloud in the presence of energy-constrained resources.

AVALON Project-Team

3. Research Program

3.1. Energy Application Profiling and Modelization

International roadmaps schedule to build exascale systems by the 2018 time frame. According to the Top500 list published in November 2013, the most powerful supercomputer is the Tianhe-2 platform, a machine with more than 3,000,000 cores. It consumes more than 17 MW for a maximum performance of 33 PFlops while the Defense Advanced Research Projects Agency (DARPA) has set to 20 MW the maximum energy consumption of an exascale supercomputer [40].

Energy efficiency is therefore a major challenge for building next generation large scale platforms. The targeted platforms will gather hundreds of million cores, low power servers, or CPUs. Besides being very important, their power consumption will be dynamic and irregular.

Thus, to consume energy efficiently, we aim at investigating two research directions. First, we need to improve the measure, the understanding, and the analysis of the large-scale platform energy consumption. Unlike approaches [41] that mix the usage of internal and external wattmeters on a small set of resources, we target high frequency and precise internal and external energy measurements of each physical and virtual resources on large scale distributed systems.

Secondly, we need to find new mechanisms that consume less and better on such platforms. Combined with hardware optimizations, several works based on shutdown or slowdown approaches aim at reducing energy consumption of distributed platforms and applications. To consume less, we first plan to explore the provision of accurate estimation of the energy consumed by applications without pre-executing and knowing them while most of the works try to do it based on in-depth application knowledge (code instrumentation [44], phase detection for specific HPC applications [49], etc.). As a second step, we aim at designing a framework model that allows interactions, dialogues and decisions taken in cooperation between the user/application, the administrator, the resource manager, and the energy supplier. While smart grid is one of the last killer scenarios for networks, electrical provisioning of next generation large IT infrastructures remains a challenge.

3.2. Data-intensive Application Profiling, Modeling, and Management

Recently, the term “Big Data” has emerged to design data sets or collections so large that they become intractable for classical tools. This term is most of the time implicitly linked to “analytics” to refer to issues such as curation, storage, search, sharing, analysis, and visualization. However, the Big Data challenge is not limited to data-analytics, a field that is well covered by programming languages and run-time systems such as Map-Reduce. It also encompasses data-intensive applications. These applications can be sorted into two categories. In High Performance Computing (HPC), data-intensive applications leverage post-petascale infrastructures to perform highly parallel computations on large amount of data, while in High Throughput Computing (HTC), a large amount of independent and sequential computations are performed on huge data collections.

These two types of data-intensive applications (HTC and HPC) raise challenges related to profiling and modeling that the Avalon team proposes to address. While the characteristics of data-intensive applications are very different, our work will remain coherent and focused. Indeed, a common goal will be to acquire a better understanding of both the applications and the underlying infrastructures running them to propose the best match between application requirements and infrastructure capacities. To achieve this objective, we will extensively rely on logging and profiling in order to design sound, accurate, and validated models. Then, the proposed models will be integrated and consolidated within a single simulation framework (SIMGRID). This will allow us to explore various potential “what-if?” scenarios and offer objective indicators to select interesting infrastructure configurations that match application specificities.

Another challenge is the ability to mix several heterogeneous infrastructures that scientists have at their disposal (*e.g.,* Grids, Clouds, and Desktop Grids) to execute data-intensive applications. Leveraging the aforementioned results, we will design strategies for efficient data management service for hybrid computing infrastructures.

3.3. Resourc-Agnostic Application Description Model

When programming in parallel, users expect to obtain performance improvement, whatever the cost is. For long, parallel machines have been simple enough to let a user program them given a minimal abstraction of their hardware. For example, MPI [43] exposes the number of nodes but hides the complexity of network topology behind a set of collective operations; OpenMP [47] simplifies the management of threads on top of a shared memory machine while OpenACC [46] aims at simplifying the use of GPGPU.

However, machines and applications are getting more and more complex so that the cost of manually handling an application is becoming very high [42]. Hardware complexity also stems from the unclear path towards next generations of hardware coming from the frequency wall: multi-core CPU, many-core CPU, GPGPUs, deep memory hierarchy, etc. have a strong impact on parallel algorithms. Hence, even though an abstract enough parallel language (UPC, Fortress, X10, etc.) succeeds, it will still face the challenge of supporting distinct codes corresponding to different algorithms corresponding to distinct hardware capacities.

Therefore, the challenge we aim to address is to define a model, for describing the structure of parallel and distributed applications that enables code variations but also efficient executions on parallel and distributed infrastructures. Indeed, this issue appears for HPC applications but also for cloud oriented applications. The challenge is to adapt an application to user constraints such as performance, energy, security, etc.

Our approach is to consider component based models [50] as they offer the ability to manipulate the software architecture of an application. To achieve our goal, we consider a “compilation” approach that transforms a resource-agnostic application description into a resource-specific description. The challenge is thus to determine a component based model that enables to efficiently compute application mapping while being tractable. In particular, it has to provide an efficient support with respect to application and resource elasticity, energy consumption and data management. OpenMP runtime is a specific use case that we target.

3.4. Application Mapping and Scheduling

This research axis is at the crossroad of the Avalon team. In particular, it gathers results of the three other research axis. We plan to consider application mapping and scheduling through the following three issues.

3.4.1. Application Mapping and Software Deployment

Application mapping and software deployment consist in the process of assigning distributed pieces of software to a set of resources. Resources can be selected according to different criteria such as performance, cost, energy consumption, security management, etc. A first issue is to select resources at application launch time. With the wide adoption of elastic platforms, *i.e.,* platforms that let the number of resources allocated to an application to be increased or decreased during its execution, the issue is also to handle resource selection at runtime.

The challenge in this context corresponds to the mapping of applications onto distributed resources. It will consist in designing algorithms that in particular take into consideration application profiling, modeling, and description.

A particular facet of this challenge is to propose scheduling algorithms for dynamic and elastic platforms. As the amount of elements can vary, some kind of control of the platforms must be used accordingly to the scheduling.

3.4.2. Non-Deterministic Workflow Scheduling

Many scientific applications are described through workflow structures. Due to the increasing level of parallelism offered by modern computing infrastructures, workflow applications now have to be composed not only of sequential programs, but also of parallel ones. New applications are now built upon workflows with conditionals and loops (also called non-deterministic workflows).

These workflows can not be scheduled beforehand. Moreover cloud platforms bring on-demand resource provisioning and pay-as-you-go billing models. Therefore, there is a problem of resource allocation for non-deterministic workflows under budget constraints and using such an elastic management of resources.

Another important issue is data management. We need to schedule the data movements and replications while taking job scheduling into account. If possible, data management and job scheduling should be done at the same time in a closely coupled interaction.

3.4.3. Security Management in Cloud Infrastructure

Security has been proven to be sometimes difficult to obtain [48] and several issues have been raised in Clouds. Nowadays virtualization is used as the sole mechanism to secure different users sharing resources on Clouds. But, due to improper virtualization of all the components of Clouds (such as micro-architectural components), data leak and modification can occur. Accordingly, next-generation protection mechanisms are required to enforce security on Clouds and provide a way to cope with the current limitation of virtualization mechanisms.

As we are dealing with parallel and distributed applications, security mechanisms must be able to cope with multiple machines. Our approach is to combine a set of existing and novel security mechanisms that are spread in the different layers and components of Clouds in order to provide an in-depth and end-to-end security on Clouds. To do it, our first challenge is to define a generic model to express security policies.

Our second challenge is to work on security-aware resource allocation algorithms. The goal of such algorithms is to find a good trade-off between security and unshared resources. Consequently, they can limit resources sharing to increase security. It leads to complex trade-off between infrastructure consolidation, performance, and security.

CIDRE Project-Team

3. Research Program

3.1. Our perspective

For many aspects of our everyday life, we heavily rely on information systems, many of which are based on massively networked devices that support a population of interacting and cooperating entities. While these information systems become increasingly open and complex, accidental and intentional failures get considerably more frequent and severe.

Two research communities traditionally address the concern of accidental and intentional failures: the distributed computing community and the security community. While both these communities are interested in the construction of systems that are correct and secure, an ideological gap and a lack of communication exist between them that is often explained by the incompatibility of the assumptions each of them traditionally makes. Furthermore, in terms of objectives, the distributed computing community has favored systems availability while the security community has focused on integrity and confidentiality, and more recently on privacy.

Our long term ambition is to contribute to the building of distributed systems that are trustworthy and respectful of privacy, even when some nodes [0] in the system have been compromised. For that purpose, we are convinced that combining classical security approaches and distributed computing paradigms is an interesting way to enforce the security of large-scale distributed systems. More specifically, since a distributed system is composed of nodes, we assert that the security of large-scale distributed systems has to be addressed at three complementary levels:

- the level of each node: each standalone node has to enforce its own security;
- the level of an *identified* set of *trusted* nodes: the *trusted* nodes can *collaborate* to enforce together their security;
- the level of fully open large-scale distributed and dynamic systems: distributed computing paradigms such as consensus algorithms can be applied to cope with the possible presence of malicious nodes.

Notice that using a distributed architecture can also be an approach allowing the nodes to enforce their security without the need of a trusted third party.

The research activities of the CIDRE project-team focus mainly on the two following research axis:

- **Intrusion Detection System:** the objective is to detect any suspicious events with regard to the security by analyzing some data generated on the monitored system.
- **Privacy-preserving Services:** the objective is to ensure users' privacy even when this property seems incompatible with the provided services, like social networks or location-based services.

In all our studies, we consider a priori that the attacker is omnipotent. He can acts as he wants. Nevertheless, being not a team specialized in cryptography, we consider that we can rely on strong unbroken cryto-systems.

3.2. Intrusion Detection / Security Events Monitoring and Management

Today, we are not yet fully entered into a world of “security by design”. Security remains often a property that is considered a posteriori, when the system is deployed, which often results in applying patches when vulnerabilities are discovered (also called a “patch and pray” approach). Unfortunately, despite patching, the number of vulnerabilities remains high, as evidenced by the number of vulnerabilities published each year in the Common Vulnerabilities and Exposures (CVE) system. Thus, it is important to be able to early detect cyber-attacks, especially when they exploit vulnerabilities that are unknown. However, the efficiency of

[0] The term node either refers to a device that hosts a network client or service or to the process that runs this client or service.

security events monitoring and management systems (including the IDS - Intrusion Detection Systems) is still an open issue today. Indeed, they are often unable to effectively deal with huge numbers of security events, and they usually produce too many false alarms yet missing some attacks. So one of the main research challenges in IT security remains the definition of efficient security events monitoring systems, i.e., that enable both to process a huge number of security events and to detect any attacks without flooding the security analysts with false alarms.

By exploiting vulnerabilities in operating systems, applications, or network services, an attacker can defeat preventive security mechanisms and violate the security policy of the whole system. The goal of an Intrusion Detection Systems (IDS) is to detect such violations by analyzing some *security events* generated on a monitored system. Ideally, the IDS should produce an alert for any violation (no *false negative*), and only for violations (no *false positive*).

To produce alerts, two detection techniques exist: the misuse based detection and the anomaly based detection. A misuse based detection is actually a signature based detection approach : it allows to detect only the attacks whose signature is available. From our point of view, while useful in practice, misuse detection is intrinsically limited. Indeed, it requires to update in real-time the database of signatures, similarly to what has to be done for antivirus tools. The CIDRE project-team follows the alternative approach, namely the anomaly approach, which consists in detecting a deviation from a referenced behavior. Our contributions on anomaly-based IDS follow three axis:

- **Illegal Information Flow Detection:** our goal is to detect information flows in the monitored system (either a node or a set of trusted nodes) that are allowed by the access control mechanism, but are illegal from the security policy point of view. This approach is particularly appealing to detect intrusions in a standalone node, such as a smartphone.
- **Anomaly-Based Detection in Distributed Applications:** our goal is to specify the normal behavior based on either a formal specification of the distributed application, or previous executions. This approach is particularly appealing to detect intrusions in industrial control systems since these systems exhibit well-defined behaviors at different levels: network level (network communication patterns, protocol specifications, etc.), control level (continue and discrete process control laws), or even the state of the local resources (memory or CPU).
- **Online data analytics:** our goal is to estimate on the fly different statistics or metrics on distributed input streams to detect abnormal behavior with respect to a well-defined criterion such as the distance between different streams, their correlation or their entropy.

Beside the anomaly-based IDS, we have also led research work on alert correlation and visualisation of security events. Indeed, in large systems, multiple (host and network) IDS and many sensors are deployed and they continuously and independently generate notifications (event's observations, warnings and alerts). To cope with this huge amount of collected data, we have studied two different approaches, each with specific goal:

- **Alert Correlation System:** the alerts of *low level* IDSes can be viewed as *security events* of a *high level* IDS whose goal is to correlate these alerts. An alert correlation system aims at exploiting the known relationships between some elements that appear in the flow of low level notifications to generate high semantic meta-alerts. The main goal is to reduce the number of alerts (and especially, false positive) returned to the security analysts and to allow a higher level analysis of the situation (situational awareness).
- **Visualization Tools:** a visualization tools aims at relying on the capacity of human beings to detect patterns and outliers in datasets when these datasets are properly visually represented. Human beings also know pieces of contextual information that are very difficult to formalize so as to make them usable by a computer. Visualization is therefore a very useful complementary tool to detect abnormal events in real time (monitoring), to search for malicious events in log files (data exploration and forensics) and to communicate results (reporting).

3.3. Privacy

In a world of ubiquitous technologies, each individual constantly leaves digital traces related to his activities and interests. The current business plan of many web services such as social networks, is based on the sale of these digital traces. Of course, this is usually done in a legal way, the license of use clearly stating that the user gives the right to the service provider for using his personal data. However, on the one hand, users generally do not read these licenses, and on the other hand, these licenses are usually very vague on the use of personal data [0]. In addition these digital traces can potentially be stolen and maliciously used, they must therefore be protected. In this context, users' privacy is now recognized as a fundamental individual right. Any new IT service should thus follow the *privacy-by-design* approach: privacy issues have to be studied from the earliest phase of a project by taking into account the multi-stakeholders and transdisciplinary aspects in order to ensure proper, end-to-end private data protection properties.

In the CIDRE project, we mainly focus on domains in which privacy issues collide with provided services. Here are some concrete examples of such domains:

- **Location-based services:** the challenge is to design services that depend on the user's location while preserving the privacy of his location;
- **Social networks:** the challenge is to demonstrate that it is possible to design social networks respectful of users' privacy;
- **Mobile services:** given that such services are based on user's identity, the challenge is to design mobile services while preserving the users' anonymity;
- **Ad-hoc netwoks:** in ad-hoc networks, any participant can potentially know the relative location of the other participants. Thus, the issue is to allow nodes to forward messages while preserving the privacy of the communications.

For all of these domains, we have proposed new Privacy-Enhancing Techniques (PETs) based on a mix of different foundations such as cryptographic techniques, security policies and access control mechanisms, just to name a few. More generally, we think that a major option to protect users' privacy consists in using a decentralized architecture that enables to transfer control and services from the service providers to the users.

The concept of IDS seems to be in contradiction with the users' privacy. Indeed, an IDS is a monitoring system that needs to collect and analyze information coming from different levels such as network, applications and OS, this information being able to include users' personal data. However, we are confident that IDS and privacy are not completely antagonist. In particular, integrating some privacy features inside an IDS to build a privacy-preserving IDS may allow to limit the amount of information that can leak if one of the nodes within the system is compromised. On the other hand, enabling IDS to detect attacks against privacy as well as security violations can extend the range of their applicability.

[0] Besides, it has been shown that service providers do not necessarily comply with their own license.

COAST Project-Team

3. Research Program

3.1. Introduction

Our scientific foundations are grounded on distributed collaborative systems supported by sophisticated data sharing mechanisms and on service oriented computing with an emphasis on orchestration and on non-functional properties.

Distributed collaborative systems enable distributed group work supported by computer technologies. Designing such systems requires an expertise in Distributed Systems and in Computer-supported collaborative Work research area. Besides theoretical and technical aspects of distributed systems, the design of distributed collaborative systems must take into account the human factor to offer solutions suitable for users and groups. The Coast team vision is to move away from a centralized authority based collaboration towards a decentralized collaboration where users have full control over their data that they can store locally and decide with whom to share them. The Coast team investigates the issues related to the management of distributed shared data and coordination between users and groups.

Service oriented Computing [26] is an established domain on which the ECOO, Score and now the Coast teams have been contributing for a long time. It refers to the general discipline that studies the development of computer applications on the web. A service is an independent software program with a specific functional context and capabilities published as a service contract (or more traditionally an API). A service composition aggregates a set of services and coordinates their interactions. The scale, the autonomy of services, the heterogeneity and some design principles underlying Service Oriented Computing open new research questions that are at the basis of our research. They span the disciplines of **distributed computing**, **software engineering** and **computer supported collaborative work** (CSCW). Our approach to contribute to the general vision of Service Oriented Computing and more generally to the emerging discipline of Service Science has been and is still to focus on the issue of the efficient and flexible construction of reliable and secure high level services through the coordination/orchestration/composition of other services provided by distributed organizations or people.

3.2. Consistency Models for Distributed Collaborative Systems

Collaborative systems are distributed systems that allow users to share data. One important issue is to manage consistency of shared data according to concurrent access. Traditional consistency criteria such as serializability, linearizability are not adequate for collaborative systems.

Causality, Convergence and Intention preservation (CCI) [30] are more suitable for developing middleware for collaborative applications.

We develop algorithms for ensuring CCI properties on collaborative distributed systems. Constraints on the algorithms are different according to the kind of distributed system and to the data structure. The distributed system can be centralized, decentralized or peer-to-peer. The type of data can include strings, growable arrays, ordered trees, semantic graphs and multimedia data.

3.3. Optimistic Replication

Replication of data among different nodes of a network allows improving reliability, fault-tolerance, and availability. When data are mutable, consistency among the different replicas must be ensured. Pessimistic replication is based on the principle of single-copy consistency while optimistic replication allows the replicas to diverge during a short time period. The consistency model for optimistic replication [28] is called eventual consistency, meaning that replicas are guaranteed to converge to the same value when the system is idle.

Our research focuses on the two most promising families of optimistic replication algorithms for ensuring CCI:

- the operational transformation (OT) algorithms [24]
- the algorithms based on commutative replicated data types (CRDT) [27].

Operational transformation algorithms are based on the application of a transformation function when a remote modification is integrated into the local document. Integration algorithms are generic, being parametrized by operational transformation functions which depend on replicated document types. The advantage of these algorithms is their genericity. These algorithms can be applied to any data type and they can merge heterogeneous data in a uniform manner.

Commutative replicated data types is a new class of algorithms initiated by WOOT [25] a first algorithm designed WithOut Operational Transformations. They ensure consistency of highly dynamic content on peer-to-peer networks. Unlike traditional optimistic replication algorithms, they can ensure consistency without concurrency control. CRDT algorithms rely on natively commutative operations defined on abstract data types such as lists or ordered trees. Thus, they do not require a merge algorithm or an integration procedure.

3.4. Process Orchestration and Management

Process Orchestration and Management is considered as a core discipline behind Service Management and Computing. It includes the analysis, the modelling, the execution, the monitoring and the continuous improvement of enterprise processes and is for us a central domain of studies.

Much efforts have been devoted in the past years to establish standard business process models founded on well grounded theories (e.g. Petri Nets) that meet the needs of both business analysts but also of software engineers and software integrators. This has lead to heated debate in the BPM community as the two points of view are very difficult to reconcile. On one side, the business people in general require models that are easy to use and understand and that can be quickly adapted to exceptional situations. On the other side, IT people need models with an operational semantic in order to be able transform them into executable artefacts. Part of our work has been an attempt to reconcile these point of views. It resulted in the development of the Bonita Business process management system and more recently on our work in crisis management where the same people are designing, executing and monitoring the process as it executes. But more generally, and at a larger scale, we have been considering the problem of processes spanning the barriers of organisations and thus more general problem of service composition as a way to coordinate inter organisational construction of applications providing value based on the composition of lower level services [22].

3.5. Service Composition

We are considering processes as pieces of software whose execution traverse the boundaries of organisations. This is especially true with service oriented computing where processes compose services produced by many organisations. We tackle this problem from very different perspectives, trying to find the best compromise between the need for privacy of internal processes from organisations and the necessity to publicize large part of them, proposing to distribute the execution and the orchestration of processes among the organisations themselves, and attempting to ensure non-functional properties in this distributed setting [21].

Non-functional aspects of service composition relate to all the properties and service agreements that one wants to ensure and that are orthogonal to the actual business but that are important when a service is selected and integrated in a composition. This includes transactional context, security, privacy, and quality of service in general. Defining and orchestrating services on a large scale while providing the stakeholders with some strong guarantees on their execution is a first class problem for us. For a long time, we have proposed models and solutions to ensure that some properties (e.g. transactional properties) were guaranteed on process execution, either through design or through the definition of some protocols. Our work has also been extended to the problems of security, privacy and service level agreement among partners. These questions are still central in our work. One major problem of current approaches is to monitor the execution of the compositions, integrating the distributed dimension. This problem can be tackled using event-based algorithms and techniques. Using our event oriented composition framework DISC, we have obtained new results dedicated to the runtime verification of violations in service choreographies.

COATI Project-Team

3. Research Program

3.1. Research Program

Members of COATI have a strong expertise in the design and management of wired and wireless backbone, backhaul, broadband, and complex networks. On the one hand, we cope with specific problems such as energy efficiency in backhaul and backbone networks, routing reconfiguration in connection oriented networks (MPLS, WDM), traffic aggregation in SONET networks, compact routing in large-scale networks, survivability to single and multiple failures, etc. These specific problems often come from questions of our industrial partners. On the other hand, we study fundamental problems mainly related to routing and reliability that appear in many networks (not restricted to our main fields of applications) and that have been widely studied in the past. However, previous solutions do not take into account the constraints of current networks/traffic such as their huge size and their dynamics. COATI thus puts a significant research effort in the following directions:

- **Energy efficiency and Software-Defined Networks (SDN)** at both the design and management levels. More precisely, we plan to study the deployment of energy-efficient routing algorithm within SDN. We developed new algorithms in order to take into account the new constraints of SDN equipments and we evaluate their performance by simulation and by experimentation on a fat-tree architecture.
- **Larger networks:** Another challenge one has to face is the increase in size of practical instances. It is already difficult, if not impossible, to solve practical instances optimally using existing tools. Therefore, we have to find new ways to solve problems using reduction and decomposition methods, characterization of polynomial instances (which are surprisingly often the practical ones), or algorithms with acceptable practical performances.
- **Stochastic behaviors:** Larger topologies mean frequent changes due to traffic and radio fluctuations, failures, maintenance operations, growth, routing policy changes, etc. We aim at including these stochastic behaviors in our combinatorial optimization process to handle the dynamics of the system and to obtain robust designs of networks.

CTRL-A Team

3. Research Program

3.1. Modeling and control techniques for autonomic computing

3.1.1. Continuous control

Continuous control was used to control computer systems only very recently and in few occasions, despite the promising results that were obtained. This is probably due to many reasons, but the most important seems to be the difficulty by both communities to transform a computer system problem into an automatic control problem. The aim of the team is to explore how to formalize typical autonomic commuting cases into typical control problems. Many new methodological tools will probably be useful for that, e.g., we can cite the hybrid system approach, predictive control or event-based control approach. Computer systems are not usual for the control system community and they often present non-conventional control aspects like saturation control. New methodological tools are required for an efficient use of continuous-time control in computer science.

3.1.2. Discrete control

Discrete control techniques are explored at long-term, to integrate more control in the BZR language, and adress more general control issues, wider than BZR's limitations. Directions are : expressiveness (taking into account in the LTS models value domains of the variables in the program) ; adaptive control (where the controller itself can dynamically switch between differents modes) ; distributed control (for classes of problems where communicating controllers can be designed) ; optimal control (w.r.t. weight functions, on states, transitions, and paths, with multicriteria techniques) ; timed and hybrid control bringing a new dimension for modeling and control, giving solutions where discrete models fail.

3.2. Design and programming for autonomic computing

3.2.1. Reactive programming

Autonomic systems are intrinsically reconfigurable. To describe, specify or design these systems, there is a need to take into account this reconfigurability, within the programming languages used. We propose to consider the reconfigurability of systems from the angle of two properties: the notion of time, as we want to describe the state and behavior of the system before, and after its reconfiguration; the notion of dynamicity of the system, i.e., considering that the system's possible behaviors throughout execution are not completely known, neither at design-time nor at initial execution state. To describe and design such reactive systems, we propose to use the synchronous paradigm. It has been successfully used, in industry, for the design of embedded systems. It allows the description of behaviors based on a specific model of time (discrete time scale, synchronous parallel composition), providing properties which are important w.r.t. the safety of the described system: reactivity, determinism, preservation of safety properties by parallel composition (with other parts of the system or with its environment). Models and languages for control, proposed in this framework, provide designers, experts of the application domain, with a user-friendly access to highly technical formal methods of DCS, by encapsulating them in the compilation of concrete programming languages, generating concrete executable code. They are based on discrete models, but also support programming of sampled continuous controllers.

3.2.2. Component-based approach and domain-specific languages

For integration of the previous control kernels into wider frameworks of reconfigurable systems, they have to be integrated in a design flow, and connected on the one side with higher-level specification languages (with help of DSLs), and on the other side with the generated code level target execution machines. This calls for the adoption of a component-based approach with necessary features, available typically in Fractal, for explicitly identifying the control interfaces and mechanisms.

Structuring and instrumentation for controllability will involve encapsulation of computations into components, specification of their local control (activation, reconfiguration, suspension, termination), and exporting appropriate interfaces (including behavior abstraction). Modeling the configurations space requires determining the controlled aspects (e.g., heterogenous CPUs loads, fault-tolerance and variability, memory, energy/power consumption, communication/bandwidth, QoS level) and their control points, as well as APIs for monitors and actions. Compilation and execution will integrate this in a complete design flow involving : extraction of a reactive model from components; instrumentation of execution platforms to be controllable; combination with other controllers; general "glue" and wrapper code.

Integration of reactive languages and control techniques in component-based systems brings interesting questions of co-existence w.r.t. other approaches like Event-Condition-Action (ECA) rules, or Complex Event Processing (CPE).

3.3. Infrastructure-level support for autonomic computing

The above general kernel of model-based control techniques can be used in a range of different computing infrastructures, representing complementary targets and abstraction levels, exploring the two axes :

- from hardware, to operating system/virtual machine, to middleware, to applications/service level;
- across different criteria for adaptation: resources and energy, quality of service, dependability.

3.3.1. Software and adaptive systems

Autonomic administration loops at operating systems or middleware level are already very widespread. An open problem remains in design techniques for controllers with predictability and safety, e.g. w.r.t. the reachable states. We want to contribute to the topic of discrete control techniques for these systems, and tackle e.g. problems of coordination of multiple autonomic loops in data-centers, as in the ANR project CtrlGreen. Another target application is the control of clusters in map-reduce applications. The objective is to use continuous time control in order to tune finely the number of required clusters for an application running on a map-reduce server. This will use results of the ANR project MyCloud that enables to simulate clients on a real map-reduce server. On a longer term, we are interested in control problems in administration loops of event-based virtual machines, or in the deployment of massively parallel computation of the Cloud.

3.3.2. Hardware and reconfigurable architectures

Reconfigurable architectures based on Field Programmable Gate Arrays (FPGA) are an active research area, where infrastructures are more and more supportive of reconfiguration, but its correct control remains an important issue. Work has begun in the ANR Famous project on identifying domain-specific control criteria and objectives, monitors and management APIs, and on integrating control techniques in the high-level RecoMARTE environment. On a longer term, we want to work on methods and tools for the programming of **multicore architectures**, exploiting the reconfigurability potentials and issues (because of variability, loss of cores), e.g. in our cooperation with ST Microelectronics, using a Fractal-based programming framework in the P2012 project, and in cooperation with Inria Lille (Adam), or with the CEA and TIMA on integrating control loops in the architecture for a fine control of the energy and of the required nodes for running a given application task.

3.3.3. Applications and autonomic systems

In autonomic systems, control systems remain a lively source of inspiration, partly because the notion of control loop implementation is known and practiced naturally. On a wider scale, we started a cooperation with Orange Labs on "intelligent" building automation and control for the Smart Grid, through modeling and control of appliances w.r.t. their power consumption modes, at home, building, and city levels. Other partners on these topics are CEA LETI/DACLE and Schneider Electric.

We could explore more systems and applications e.g., Human-Machine Interfaces, or the orchestration of services. They can help design more general solutions, and result in a more complete methodology.

DANTE Project-Team

3. Research Program

3.1. Graph-based signal processing

Participants: Christophe Crespelle, Éric Fleury, Paulo Gonçalves Andrade, Márton Karsai, Sarah de Nigris, Sarra Ben Alaya, Hadrien Hours.

Evolving networks can be regarded as "*out of equilibrium*" systems. Indeed, their dynamics is typically characterized by non standard and intricate statistical properties, such as non-stationarity, long range memory effects, intricate space and time correlations.

Analyzing, modeling, and even defining adapted concepts for dynamic graphs is at the heart of DANTE. This is a largely open question that has to be answered by keeping a balance between specificity (solutions triggered by specific data sets) and generality (universal approaches disconnected from social realities). We will tackle this challenge from a graph-based signal processing perspective involving signal analysts and computer scientists, together with experts of the data domain application. One can distinguish two different issues in this challenge, one related to the graph-based organisation of the data and the other to the time dependency that naturally exits in the dynamic graph object. In both cases, a number of contributions can be found in the literature, albeit in different contexts. In our application domain, high-dimensional data "naturally reside" on the vertices of weighted graphs. The emerging field of signal processing on graphs merges algebraic and spectral graph theoretic concepts with computational harmonic analysis to process such signals on graphs [70].

As for the first point, adapting well-founded signal processing techniques to data represented as graphs is an emerging, yet quickly developing field which has already received key contributions. Some of them are very general and delineate ambitious programs aimed at defining universal, generally unsupervised methods for exploring high-dimensional data sets and processing them. This is the case for instance of the Â« diffusion wavelets Â» and Â« diffusion maps Â» pushed forward at Yale and Duke [54]. Others are more traditionally connected with standard signal processing concepts, in the spirit of elaborating new methodologies via some bridging between networks and time series, see, *e.g.*, ([65] and references therein). Other viewpoints can be found as well, including multi-resolution Markov models [73], Bayesian networks or distributed processing over sensor networks [64]. Such approaches can be particularly successful for handling static graphs and unveiling aspects of their organisation in terms of dependencies between nodes, grouping, etc. Incorporating possible time dependencies within the whole picture calls however for the addition of an extra dimension to the problem "as it would be the case when switching from one image to a video sequence", a situation for which one can imagine to take advantage of the whole body of knowledge attached to non-stationary signal processing [55].

3.2. Theory and Structure of dynamic Networks

Participants: Christophe Crespelle, Éric Fleury, Anthony Busson, Márton Karsai.

Characterization of the dynamics of complex networks. We need to focus on intrinsic properties of evolving/dynamic complex networks. New notions (as opposed to classical static graph properties) have to be introduced: rate of vertices or links appearances or disappearances, the duration of link presences or absences. Moreover, more specific properties related to the dynamics have to be defined and are somehow related to the way to model a dynamic graph.

Through the systematic analysis and characterization of static network representations of many different systems, researchers of several disciplines have unveiled complex topologies and heterogeneous structures, with connectivity patterns statistically characterized by heavy-tails and large fluctuations, scale-free properties and non trivial correlations such as high clustering and hierarchical ordering [67]. A large amount of work has been devoted to the development of new tools for statistical characterisation and modelling of networks, in order to identify their most relevant properties, and to understand which growth mechanisms could lead to these properties. Most of those contributions have focused on static graphs or on dynamic process (*e.g.* diffusion) occurring on static graphs. This has called forth a major effort in developing the methodology to characterize the topology and temporal behavior of complex networks [67], [58], [74], [63], to describe the observed structural and temporal heterogeneities [52], [58], [53], to detect and measure emerging community structures [56], [71], [72], to see how the functionality of networks determines their evolving structure [62], and to determine what kinds of correlations play a role in their dynamics [59], [61], [66].

The challenge is now to extend this kind of statistical characterization to dynamical graphs. In other words, links in dynamic networks are temporal events, called contacts, which can be either punctual or last for some period of time. Because of the complexity of this analysis, the temporal dimension of the network is often ignored or only roughly considered. Therefore, fully taking into account the dynamics of the links into a network is a crucial and highly challenging issue.

Another powerful approach to model time-varying graphs is via activity driven network models. In this case, the only assumption relates to the distribution of activity rates of interacting entities. The activity rate is realistically broadly distributed and refers to the probability that an entity becomes active and creates a connection with another entity within a unit time step [69]. Even the generic model is already capable to recover some realistic features of the emerging graph, its main advantage is to provide a general framework to study various types of correlations present in real temporal networks. By synthesizing such correlations (*e.g.* memory effects, preferential attachment, triangular closing mechanisms, ...) from the real data, we are able to extend the general mechanism and build a temporal network model, which shows certain realistic feature in a controlled way. This can be used to study the effect of selected correlations on the evolution of the emerging structure [60] and its co-evolution with ongoing processes like spreading phenomena, synchronisation, evolution of consensus, random walk etc. [60], [68]. This approach allows also to develop control and immunisation strategies by fully considering the temporal nature of the backgrounding network.

3.3. Distributed Algorithms for dynamic networks: regulation, adaptation and interaction

Participants: Thomas Begin, Anthony Busson, Paulo Gonçalves Andrade, Isabelle Guérin Lassous.

Dedicated algorithms for dynamic networks. First, the dynamic network object itself trigger original algorithmic questions. It mainly concerns distributed algorithms that should be designed and deployed to efficiently measure the object itself and get an accurate view of its dynamic behavior. Such distributed measure should be "transparent", that is, it should introduce no bias or at least a bias that is controllable and corrigible. Such problem is encountered in all distributed metrology measures / distributed probes: P2P, sensor network, wireless network, QoS routing... This question raises naturally the intrinsic notion of adaptation and control of the dynamic network itself since it appears that autonomous networks and traffic aware routing are becoming crucial.

Communication networks are dynamic networks that potentially undergo high dynamicity. The dynamicity exhibited by these networks results from several factors including, for instance, changes in the topology and varying workload conditions. Although most implemented protocols and existing solutions in the literature can cope with a dynamic behavior, the evolution of their behavior operates identically whatever the actual properties of the dynamicity. For instance, parameters of the routing protocols (*e.g.* hello packets transmission frequency) or routing methods (*e.g.* reactive / proactive) are commonly hold constant regardless of the nodes mobility. Similarly, the algorithms ruling CSMA/CA (*e.g.* size of the contention window) are tuned identically and they do not change according to the actual workload and observed topology.

Dynamicity in computer networks tends to affect a large number of performance parameters (if not all) coming from various layers (viz. physical, link, routing and transport). To find out which ones matter the most for our intended purpose, we expect to rely on the tools developed by the two former axes. These quantities should capture and characterize the actual network dynamicity. Our goal is to take advantage of this latter information in order to refine existing protocols, or even to propose new solutions. More precisely, we will attempt to associate "fundamental" changes occurring in the underlying graph of a network (reported through graph-based signal tools) to quantitative performance that are matter of interests for networking applications and the end-users. We expect to rely on available testbeds such as Senslab and FIT to experiment our solutions and ultimately validate our approach.

DATAMOVE Team

3. Research Program

3.1. Motivation

Today's largest supercomputers [0] are composed of few millions of cores, with performances almost reaching 100 PetaFlops [0] for the largest machine. Moving data in such large supercomputers is becoming a major performance bottleneck, and the situation is expected to worsen even more at exascale and beyond. The data transfer capabilities are growing at a slower rate than processing power ones. The profusion of available flops will very likely be underused due to constrained communication capabilities. It is commonly admitted that data movements account for 50% to 70% of the global power consumption [0]. Thus, data movements are potentially one of the most important source of savings for enabling supercomputers to stay in the commonly adopted energy barrier of 20 MegaWatts. In the mid to long term, non volatile memory (NVRAM) is expected to deeply change the machine I/Os. Data distribution will shift from disk arrays with an access time often considered as uniform, towards permanent storage capabilities at each node of the machine, making data locality an even more prevalent paradigm.

The DataMove team works on **optimizing data movements for large scale computing** mainly at two related levels:

- Resource allocation
- Integration of numerical simulation and data analysis

The resource and job management system (also called batch scheduler or RJMS) is in charge of allocating resources upon user requests for executing their parallel applications. The growing cost of data movements requires adapted scheduling policies able to take into account the influence of intra-application communications, I/Os as well as contention caused by data traffic generated by other concurrent applications. Modelling the application behavior to anticipate its actual resource usage on such architecture is known to be challenging, but it becomes critical for improving performances (execution time, energy, or any other relevant objective). The job management system also needs to handle new types of workloads: high performance platforms now need to execute more and more often data intensive processing tasks like data analysis in addition to traditional computation intensive numerical simulations. In particular, the ever growing amount of data generated by numerical simulation calls for a tighter integration between the simulation and the data analysis. The challenge here is to reduce data traffic and to speed-up result analysis by performing result processing (compression, indexation, analysis, visualization, etc.) as closely as possible to the locus and time of data generation. This emerging trend called *in situ analytics* requires to revisit the traditional workflow (loop of batch processing followed by postmortem analysis). The application becomes a whole including the simulation, in situ processing and I/Os. This motivates the development of new well-adapted resource sharing strategies, data structures and parallel analytics schemes to efficiently interleave the different components of the application and globally improve the performance.

3.2. Strategy

DataMove targets HPC (High Performance Computing) at Exascale. But such machines and the associated applications are expected to be available only in 5 to 10 years. Meanwhile, we expect to see a growing number of petaflop machines to answer the needs for advanced numerical simulations. A sustainable exploitation of these petaflop machines is a real and hard challenge that we address. We may also see in the coming years a convergence between HPC and Big Data, HPC platforms becoming more elastic and supporting Big Data

[0] Top500 Ranking, http://www.top500.org

[0] 10^{15} floating point operations per second

[0] SciDAC Review, 2010, http://www.scidacreview.org/1001/pdf/hardware.pdf

jobs, or HPC applications being more commonly executed on cloud like architectures. This is the second top objective of the 2015 US Strategic Computing Initiative [0]: *Increasing coherence between the technology base used for modelling and simulation and that used for data analytic computing*. We contribute to that convergence at our level, considering more dynamic and versatile target platforms and types of workloads.

Our approaches should entail minimal modifications on the code of numerical simulations. Often large scale numerical simulations are complex domain specific codes with a long life span. We assume these codes as being sufficiently optimized. We influence the behavior of numerical simulations through resource allocation at the job management system level or when interleaving them with analytics code.

To tackle these issues, we propose to intertwine theoretical research and practical developments in an agile mode. Algorithms with performance guarantees are designed and experimented on large scale platforms with realistic usage scenarios developed with partner scientists or based on logs of the biggest available computing platforms (national supercomputers like Curie, or the BlueWaters machine accessible through our collaboration with Argonne National Lab). Conversely, a strong experimental expertise enables to feed theoretical models with sound hypotheses, to twist proven algorithms with practical heuristics that could be further retro-feeded into adequate theoretical models.

A central scientific question is to make the relevant choices for optimizing performance (in a broad sense) in a reasonable time. HPC architectures and applications are increasingly complex systems (heterogeneity, dynamicity, uncertainties), which leads to consider the **optimization of resource allocation based on multiple objectives**, often contradictory (like energy and run-time for instance). Focusing on the optimization of one particular objective usually leads to worsen the others. The historical positioning of some members of the team who are specialists in multi-objective optimization is to generate a (limited) set of trade-off configurations, called *Pareto points*, and choose when required the most suitable trade-off between all the objectives. This methodology differs from the classical approaches, which simplify the problem into a single objective one (focus on a particular objective, combining the various objectives or agglomerate them). The real challenge is thus to combine algorithmic techniques to account for this diversity while guaranteeing a target efficiency for all the various objectives.

The DataMove team aims to elaborate generic and effective solutions of practical interest. We make our new algorithms accessible through the team flagship software tools, **the OAR batch scheduler and the in situ processing framework FlowVR**. We maintain and enforce strong links with teams closely connected with large architecture design and operation, as well as scientists of other disciplines, in particular computational biologists, with whom we elaborate and validate new usage scenarios.

3.3. Research Directions

DataMove targets HPC (High Performance Computing) at Exascale. But such machines and the associated applications are expected to be available only in 5 to 10 years. Meanwhile, we expect to see a growing number of petaflop machines to answer the needs for advanced numerical simulations. A sustainable exploitation of these petaflop machines is a real and hard challenge that we address. We may also see in the coming years a convergence between HPC and Big Data, HPC platforms becoming more elastic and supporting Big Data jobs, or HPC applications being more commonly executed on cloud like architectures. This is the second top objective of the 2015 US Strategic Computing Initiative [0]: *Increasing coherence between the technology base used for modelling and simulation and that used for data analytic computing*. We contribute to that convergence at our level, considering more dynamic and versatile target platforms and types of workloads.

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[0] https://www.whitehouse.gov/the-press-office/2015/07/29/executive-order-creating-national-strategic-computing-initiative

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DIANA Project-Team

3. Research Program

3.1. Service Transparency

Transparency is to provide network users and application developers with reliable information about the current or predicted quality of their communication services, and about potential leakages of personal information, or of other information related to societal interests of the user as a "connected citizen" (e.g. possible violation of network neutrality, opinion manipulation). Service transparency therefore means to provide information meaningful to users and application developers, such as quality of experience, privacy leakages, or opinion manipulation, etc. rather than network-level metrics such as available bandwidth, loss rate, delay or jitter.

The Internet is built around a best effort routing service that does not provide any guarantee to end users in terms of quality of service (QoS). The simplicity of the Internet routing service is at the root of its huge success. Unfortunately, a simple service means unpredicted quality at the access. Even though a considerable effort is done by operators and content providers to optimise the Internet content delivery chain, mainly by over-provisioning and sophisticated engineering techniques, service degradation is still part of the Internet. The proliferation of wireless and mobile access technologies, and the versatile nature of Internet traffic, make end users quality of experience (QoE) forecast even harder. As a matter of fact, the Internet is missing a dedicated measurement plane that informs the end users on the quality they obtain and in case of substantial service degradation, on the origin of this degradation. Current state of the art activities are devoted to building a distributed measurement infrastructure to perform active, passive and hybrid measurements in the wired Internet. However, the problem is exacerbated with modern terminals such as smartphones or tablets that do not facilitate the task for end users (they even make it harder) as they focus on simplifying the interface and limiting the control on the network, whereas the Internet behind is still the same in terms of the quality it provides. Interestingly, this same observation explains the existing difficulty to detect and prevent privacy leaks. We argue that the lack of transparency for diagnosing QoE and for detecting privacy leaks have the same root causes and can be solved using common primitives. For instance, in both cases, it is important to be able to link data packets to an application. Indeed, as the network can only access data packets, there must be a way to bind these packets to an application (to understand users QoE for this application or to associate a privacy leak to an application). This is however a complex task as the traffic might be obfuscated or encrypted. Our objectives in the research direction are the following:

- Design and develop measurement tools providing transparency, in spite of current complexity
- Deploy those measurement tools at the Internet's edge and make them useful for end users
- Propose measurements plane as an overlay or by exploiting in-network functionalities
- Adapt measurements techniques to network architectural change
- Provide measurements as native functionality in future network architecture

3.2. Open network architecture

We are surrounded by personal content of all types: photos, videos, documents, etc. The volume of such content is increasing at a fast rate, and at the same time, the spread of such content among all our connected devices (mobiles, storage devices, set-top boxes, etc) is also increasing. All this complicates the control of personal content by the user both in terms of access and sharing with other users. The access of the personal content in a seamless way independently of its location is a key challenge for the future of networks. Proprietary solutions exist, but apart from fully depending on one of them, there is no standard plane in the Internet for a seamless access to personal content. Therefore, providing network architectural support to design and develop content access and sharing mechanisms is crucial to allow users control their own data over heterogeneous underlying network or cloud services.

On the other hand, privacy is a growing concern for states, administrations, and companies. Indeed, for instance the French CNIL (entity in charge of citizens privacy in computer systems) puts privacy at the core of its activities by defining rules on any stored and collected private data. Also, companies start to use privacy preserving solutions as a competitive advantage. Therefore, understanding privacy leaks and preventing them is a problem that can already find support. However, all end-users do not *currently* put privacy as their first concern. Indeed, in face of two services with one of higher quality, they usually prefer the highest quality one whatever the privacy implication. This was, for instance, the case concerning the Web search service of Google that is more accurate but less privacy preserving than Bing. This is also the case for cloud services such as iCloud or Dropbox that are much more convenient than open source solutions, but very bad in terms of privacy. Therefore, to reach end-users, any privacy preserving solutions must offer a service equivalent to the best existing services.

We consider that it will be highly desirable for Internet users to be able to *easily* move their content from a provider to another and therefore not to depend on a content provider or a social network monopoly. This requires that the network provides built-in architectural support for content networking.

In this research direction, we will define a new *service abstraction layer* (SAL) that could become the new waist of the network architecture with network functionalities below (IP, SDN, cloud) and applications on top. SAL will define different services that are of use to all Internet users for accessing and sharing data (seamless content localisation and retrieval, privacy leakage protection, transparent vertical and horizontal handover, etc.). The biggest challenge here is to cope in the same time with large number of content applications requirements and high underlying networks heterogeneity while still providing efficient applications performance. This requires careful definition of the services primitives and the parameters to be exchanged through the service abstraction layer.

Two concurring factors make the concept behind SAL feasible and relevant today. First, the notion of scalable network virtualization that is a required feature to deploy SAL in real networks today has been discussed recently only. Second, the need for new services abstraction is recent. Indeed, fifteen years ago the Internet for the end-users was mostly the Web. Only eight years ago smartphones came into the picture of the Internet boosting the number of applications with new functionalities and risks. Since a few years, many discussions in the network communities took place around the actual complexity of the Internet and the difficulty to develop applications. Many different approaches have been discussed (such as CCN, SDN) that intend to solve only part of the complexity. SAL takes a broader architectural look at the problem and considers solutions such as CCN as mere use cases. Our objectives in this research direction include the following:

- Identify common key networking services required for content access and sharing
- Detect and prevent privacy leaks for content communication
- Enhance software defined networks for large scale heterogeneous environments
- Design and develop open Content Networking architecture
- Define a service abstraction layer as the thin waist for the future content network architecture
- Test and deploy different applications using SAL primitives on heterogeneous network technologies

3.3. Methodology

We follow an experimental approach that can be described in the following techniques:

- Measurements: the aim is to get a better view of a problem in quantifiable terms. Depending on the field of interest, this may involve large scale distributed systems crawling tools; active probing techniques to infer the status and properties of a complex and non controllable system as the Internet; or even crowdsourcing-based deployments for gathering data on real-users environments or behaviours.
- Experimental evaluation: once a new idea has been designed and implemented, it is of course very desirable to assess and quantify how effective it can be, before being able to deploy it on any realistic scale. This is why a wide range of techniques can be considered for getting early, yet as significant as possible, feedback on a given paradigm or implementation. The spectrum for such techniques span from simulations to real deployments in protected and/or controlled environments.

DIONYSOS Project-Team

3. Research Program

3.1. Introduction

The scientific foundations of our work are those of network design and network analysis. Specifically, this concerns the principles of packet switching and in particular of IP networks (protocol design, protocol testing, routing, scheduling techniques), and the mathematical and algorithmic aspects of the associated problems, on which our methods and tools are based.

These foundations are described in the following paragraphs. We begin by a subsection dedicated to Quality of Service (QoS) and Quality of Experience (QoE), since they can be seen as unifying concepts in our activities. Then we briefly describe the specific sub-area of model evaluation and about the particular multidisciplinary domain of network economics.

3.2. Quality of Service and Quality of Experience

Since it is difficult to develop as many communication solutions as possible applications, the scientific and technological communities aim towards providing general *services* allowing to give to each application or user a set of properties nowadays called "Quality of Service" (QoS), a terminology lacking a precise definition. This QoS concept takes different forms according to the type of communication service and the aspects which matter for a given application: for performance it comes through specific metrics (delays, jitter, throughput, etc.), for dependability it also comes through appropriate metrics: reliability, availability, or vulnerability, in the case for instance of WAN (Wide Area Network) topologies, etc.

QoS is at the heart of our research activities: We look for methods to obtain specific "levels" of QoS and for techniques to evaluate the associated metrics. Our ultimate goal is to provide tools (mathematical tools and/or algorithms, under appropriate software "containers" or not) allowing users and/or applications to attain specific levels of QoS, or to improve the provided QoS, if we think of a particular system, with an optimal use of the resources available. Obtaining a good QoS level is a very general objective. It leads to many different areas, depending on the systems, applications and specific goals being considered. Our team works on several of these areas. We also investigate the impact of network QoS on multimedia payloads to reduce the impact of congestion.

Some important aspects of the behavior of modern communication systems have subjective components: the quality of a video stream or an audio signal, *as perceived by the user*, is related to some of the previous mentioned parameters (packet loss, delays, ...) but in an extremely complex way. We are interested in analyzing these types of flows from this user-oriented point of view. We focus on the *user perceived quality*, in short, PQ, the main component of what is nowadays called Quality of Experience (in short, QoE), to underline the fact that, in this case, we want to center the analysis on the user. In this context, we have a global project called PSQA, which stands for Pseudo-Subjective Quality Assessment, and which refers to a technology we have developed allowing to automatically measure this PQ.

Another special case to which we devote research efforts in the team is the analysis of qualitative properties related to interoperability assessment. This refers to the act of determining if end-to-end functionality between at least two communicating systems is as required by the base standards for those systems. Conformance is the act of determining to what extent a single component conforms to the individual requirements of the standard it is based on. Our purpose is to provide such a formal framework (methods, algorithms and tools) for interoperability assessment, in order to help in obtaining efficient interoperability test suites for new generation networks, mainly around IPv6-related protocols. The interoperability test suites generation is based on specifications (standards and/or RFCs) of network components and protocols to be tested.

3.3. Stochastic modeling

The scientific foundations of our modeling activities are composed of stochastic processes theory and, in particular, Markov processes, queuing theory, stochastic graphs theory, etc. The objectives are either to develop numerical solutions, or analytical ones, or possibly discrete event simulation or Monte Carlo (and Quasi-Monte Carlo) techniques. We are always interested in model evaluation techniques for dependability and performability analysis, both in static (network reliability) and dynamic contexts (depending on the fact that time plays an explicit role in the analysis or not). We look at systems from the classical so-called *call level*, leading to standard models (for instance, queues or networks of queues) and also at the *burst level*, leading to *fluid models*.

In recent years, our work on the design of the topologies of WANs led us to explore optimization techniques, in particular in the case of very large optimization problems, usually formulated in terms of graphs. The associated methods we are interested in are composed of simulated annealing, genetic algorithms, TABU search, etc. For the time being, we have obtained our best results with GRASP techniques.

Network pricing is a good example of a multi-disciplinary research activity half-way between applied mathematics, economy and networking, centered on stochastic modeling issues. Indeed, the Internet is facing a tremendous increase of its traffic volume. As a consequence, real users complain that large data transfers take too long, without any possibility to improve this by themselves (by paying more, for instance). A possible solution to cope with congestion is to increase the link capacities; however, many authors consider that this is not a viable solution as the network must respond to an increasing demand (and experience has shown that demand of bandwidth has always been ahead of supply), especially now that the Internet is becoming a commercial network. Furthermore, incentives for a fair utilization between customers are not included in the current Internet. For these reasons, it has been suggested that the current flat-rate fees, where customers pay a subscription and obtain an unlimited usage, should be replaced by usage-based fees. Besides, the future Internet will carry heterogeneous flows such as video, voice, email, web, file transfers and remote login among others. Each of these applications requires a different level of QoS: for example, video needs very small delays and packet losses, voice requires small delays but can afford some packet losses, email can afford delay (within a given bound) while file transfer needs a good average throughput and remote login requires small round-trip times. Some pricing incentives should exist so that each user does not always choose the best QoS for her application and so that the final result is a fair utilization of the bandwidth. On the other hand, we need to be aware of the trade-off between engineering efficiency and economic efficiency; for example, traffic measurements can help in improving the management of the network but is a costly option. These are some of the various aspects often present in the pricing problems we address in our work. More recently, we have switched to the more general field of network economics, dealing with the economic behavior of users, service providers and content providers, as well as their relations.

DIVERSE Project-Team

3. Research Program

3.1. Scientific background

3.1.1. Model-driven engineering

Model-Driven Engineering (MDE) aims at reducing the accidental complexity associated with developing complex software-intensive systems (e.g., use of abstractions of the problem space rather than abstractions of the solution space) [117]. It provides DIVERSE with solid foundations to specify, analyze and reason about the different forms of diversity that occur through the development lifecycle. A primary source of accidental complexity is the wide gap between the concepts used by domain experts and the low-level abstractions provided by general-purpose programming languages [88]. MDE approaches address this problem through modeling techniques that support separation of concerns and automated generation of major system artifacts from models (*e.g.,* test cases, implementations, deployment and configuration scripts). In MDE, a model describes an aspect of a system and is typically created or derived for specific development purposes [70]. Separation of concerns is supported through the use of different modeling languages, each providing constructs based on abstractions that are specific to an aspect of a system. MDE technologies also provide support for manipulating models, for example, support for querying, slicing, transforming, merging, and analyzing (including executing) models. Modeling languages are thus at the core of MDE, which participates to the development of a sound *Software Language Engineering*[0], including an unified typing theory that integrate models as first class entities [120].

Incorporating domain-specific concepts and high-quality development experience into MDE technologies can significantly improve developer productivity and system quality. Since the late nineties, this realization has led to work on MDE language workbenches that support the development of domain-specific modeling languages (DSMLs) and associated tools (*e.g.,* model editors and code generators). A DSML provides a bridge between the field in which domain experts work and the implementation (programming) field. Domains in which DSMLs have been developed and used include, among others, automotive, avionics, and the emerging cyber-physical systems. A study performed by Hutchinson et al. [94] provides some indications that DSMLs can pave the way for wider industrial adoption of MDE.

More recently, the emergence of new classes of systems that are complex and operate in heterogeneous and rapidly changing environments raises new challenges for the software engineering community. These systems must be adaptable, flexible, reconfigurable and, increasingly, self-managing. Such characteristics make systems more prone to failure when running and thus the development and study of appropriate mechanisms for continuous design and run-time validation and monitoring are needed. In the MDE community, research is focused primarily on using models at design, implementation, and deployment stages of development. This work has been highly productive, with several techniques now entering a commercialization phase. As software systems are becoming more and more dynamic, the use of model-driven techniques for validating and monitoring run-time behavior is extremely promising [102].

3.1.2. Variability modeling

While the basic vision underlying *Software Product Lines* (SPL) can probably be traced back to David Parnas seminal article [110] on the Design and Development of Program Families, it is only quite recently that SPLs are emerging as a paradigm shift towards modeling and developing software system families rather than individual systems [108]. SPL engineering embraces the ideas of mass customization and software reuse. It focuses on the means of efficiently producing and maintaining multiple related software products, exploiting what they have in common and managing what varies among them.

[0] See http://planet-sl.org

Several definitions of the *software product line* concept can be found in the research literature. Clements *et al.* define it as *a set of software-intensive systems sharing a common, managed set of features that satisfy the specific needs of a particular market segment or mission and are developed from a common set of core assets in a prescribed way* [107]. Bosch provides a different definition [76]: *A SPL consists of a product line architecture and a set of reusable components designed for incorporation into the product line architecture. In addition, the PL consists of the software products developed using the mentioned reusable assets*. In spite of the similarities, these definitions provide different perspectives of the concept: *market-driven*, as seen by Clements *et al.*, and *technology-oriented* for Bosch.

SPL engineering is a process focusing on capturing the *commonalities* (assumptions true for each family member) and *variability* (assumptions about how individual family members differ) between several software products [82]. Instead of describing a single software system, a SPL model describes a set of products in the same domain. This is accomplished by distinguishing between elements common to all SPL members, and those that may vary from one product to another. Reuse of core assets, which form the basis of the product line, is key to productivity and quality gains. These core assets extend beyond simple code reuse and may include the architecture, software components, domain models, requirements statements, documentation, test plans or test cases.

The SPL engineering process consists of two major steps:

1. **Domain Engineering**, or *development for reuse*, focuses on core assets development.
2. **Application Engineering**, or *development with reuse*, addresses the development of the final products using core assets and following customer requirements.

Central to both processes is the management of **variability** across the product line [90]. In common language use, the term *variability* refers to *the ability or the tendency to change*. Variability management is thus seen as the key feature that distinguishes SPL engineering from other software development approaches [77]. Variability management is thus growingly seen as the cornerstone of SPL development, covering the entire development life cycle, from requirements elicitation [122] to product derivation [127] to product testing [106], [105].

Halmans *et al.* [90] distinguish between *essential* and *technical* variability, especially at requirements level. Essential variability corresponds to the customer's viewpoint, defining what to implement, while technical variability relates to product family engineering, defining how to implement it. A classification based on the dimensions of variability is proposed by Pohl *et al.* [112]: beyond **variability in time** (existence of different versions of an artifact that are valid at different times) and **variability in space** (existence of an artifact in different shapes at the same time) Pohl *et al.* claim that variability is important to different stakeholders and thus has different levels of visibility: **external variability** is visible to the customers while **internal variability**, that of domain artifacts, is hidden from them. Other classification proposals come from Meekel *et al.* [100] (feature, hardware platform, performances and attributes variability) or Bass *et al.* [68] who discuss about variability at the architectural level.

Central to the modeling of variability is the notion of *feature*, originally defined by Kang *et al.* as: *a prominent or distinctive user-visible aspect, quality or characteristic of a software system or systems* [96]. Based on this notion of *feature*, they proposed to use a *feature model* to model the variability in a SPL. A feature model consists of a *feature diagram* and other associated information: *constraints* and *dependency rules*. Feature diagrams provide a *graphical tree-like notation depicting the hierarchical organization of high level product functionalities* represented as features. The root of the tree refers to the complete system and is progressively decomposed into more refined features (tree nodes). Relations between nodes (features) are materialized by *decomposition edges* and *textual constraints*. Variability can be expressed in several ways. Presence or absence of a feature from a product is modeled using *mandatory* or *optional features*. Features are graphically represented as rectangles while some graphical elements (e.g., unfilled circle) are used to describe the variability (e.g., a feature may be optional).

Features can be organized into *feature groups*. Boolean operators *exclusive alternative (XOR)*, *inclusive alternative (OR)* or *inclusive (AND)* are used to select one, several or all the features from a feature group.

Dependencies between features can be modeled using *textual constraints*: *requires* (presence of a feature requires the presence of another), *mutex* (presence of a feature automatically excludes another). Feature attributes can be also used for modeling quantitative (e.g., numerical) information. Constraints over attributes and features can be specified as well.

Modeling variability allows an organization to capture and select which version of which variant of any particular aspect is wanted in the system [77]. To implement it cheaply, quickly and safely, redoing by hand the tedious weaving of every aspect is not an option: some form of automation is needed to leverage the modeling of variability [72], [84]. Model Driven Engineering (MDE) makes it possible to automate this weaving process [95]. This requires that models are no longer informal, and that the weaving process is itself described as a program (which is as a matter of facts an executable meta-model [103]) manipulating these models to produce for instance a detailed design that can ultimately be transformed to code, or to test suites [111], or other software artifacts.

3.1.3. Component-based software development

Component-based software development [121] aims at providing reliable software architectures with a low cost of design. Components are now used routinely in many domains of software system designs: distributed systems, user interaction, product lines, embedded systems, etc. With respect to more traditional software artifacts (e.g., object oriented architectures), modern component models have the following distinctive features [83]: description of requirements on services required from the other components; indirect connections between components thanks to ports and connectors constructs [98]; hierarchical definition of components (assemblies of components can define new component types); connectors supporting various communication semantics [80]; quantitative properties on the services [75].

In recent years component-based architectures have evolved from static designs to dynamic, adaptive designs (e.g., SOFA [80], Palladio [73], Frascati [104]). Processes for building a system using a statically designed architecture are made of the following sequential lifecycle stages: requirements, modeling, implementation, packaging, deployment, system launch, system execution, system shutdown and system removal. If for any reason after design time architectural changes are needed after system launch (e.g., because requirements changed, or the implementation platform has evolved, etc) then the design process must be reexecuted from scratch (unless the changes are limited to parameter adjustment in the components deployed).

Dynamic designs allow for *on the fly* redesign of a component based system. A process for dynamic adaptation is able to reapply the design phases while the system is up and running, without stopping it (this is different from stop/redeploy/start). This kind of process supports *chosen adaptation*, when changes are planned and realized to maintain a good fit between the needs that the system must support and the way it supports them [97]. Dynamic component-based designs rely on a component meta-model that supports complex life cycles for components, connectors, service specification, etc. Advanced dynamic designs can also take platform changes into account at run-time, without human intervention, by adapting themselves [81], [124]. Platform changes and more generally environmental changes trigger *imposed adaptation*, when the system can no longer use its design to provide the services it must support. In order to support an eternal system [74], dynamic component based systems must separate architectural design and platform compatibility. This requires support for heterogeneity, since platform evolutions can be partial.

The Models@runtime paradigm denotes a model-driven approach aiming at taming the complexity of dynamic software systems. It basically pushes the idea of reflection one step further by considering the reflection layer as a real model “something simpler, safer or cheaper than reality to avoid the complexity, danger and irreversibility of reality [115]”. In practice, component-based (and/or service-based) platforms offer reflection APIs that make it possible to introspect the system (which components and bindings are currently in place in the system) and dynamic adaptation (by applying CRUD operations on these components and bindings). While some of these platforms offer rollback mechanisms to recover after an erroneous adaptation, the idea of Models@runtime is to prevent the system from actually enacting an erroneous adaptation. In other words, the “model at run-time” is a reflection model that can be uncoupled (for reasoning, validation, simulation purposes) and automatically resynchronized.

Heterogeneity is a key challenge for modern component based system. Until recently, component based techniques were designed to address a specific domain, such as embedded software for command and control, or distributed Web based service oriented architectures. The emergence of the Internet of Things paradigm calls for a unified approach in component based design techniques. By implementing an efficient separation of concern between platform independent architecture management and platform dependent implementations, *Models@runtime* is now established as a key technique to support dynamic component based designs. It provides DIVERSE with an essential foundation to explore an adaptation envelop at run-time.

Search Based Software Engineering [92] has been applied to various software engineering problems in order to support software developers in their daily work. The goal is to automatically explore a set of alternatives and assess their relevance with respect to the considered problem. These techniques have been applied to craft software architecture exhibiting high quality of services properties [89]. Multi Objectives Search based techniques [86] deal with optimization problem containing several (possibly conflicting) dimensions to optimize. These techniques provide DIVERSE with the scientific foundations for reasoning and efficiently exploring an envelope of software configurations at run-time.

3.1.4. Validation and verification

Validation and verification (V&V) theories and techniques provide the means to assess the validity of a software system with respect to a specific correctness envelop. As such, they form an essential element of DIVERSE's scientific background. In particular, we focus on model-based V&V in order to leverage the different models that specify the envelop at different moments of the software development lifecycle.

Model-based testing consists in analyzing a formal model of a system (*e.g.*, activity diagrams, which capture high-level requirements about the system, statecharts, which capture the expected behavior of a software module, or a feature model, which describes all possible variants of the system) in order to generate test cases that will be executed against the system. Model-based testing [123] mainly relies on model analysis, constraint solving [85] and search-based reasoning [99]. DIVERSE leverages in particular the applications of model-based testing in the context of highly-configurable systems and [125] interactive systems [101] as well as recent advances based on diversity for test cases selection [93].

Nowadays, it is possible to simulate various kinds of models. Existing tools range from industrial tools such as Simulink, Rhapsody or Telelogic to academic approaches like Omega [109], or Xholon [0]. All these simulation environments operate on homogeneous environment models. However, to handle diversity in software systems, we also leverage recent advances in heterogeneous simulation. Ptolemy [79] proposes a common abstract syntax, which represents the description of the model structure. These elements can be decorated using different directors that reflect the application of a specific model of computation on the model element. Metropolis [69] provides modeling elements amenable to semantically equivalent mathematical models. Metropolis offers a precise semantics flexible enough to support different models of computation. ModHel'X [91] studies the composition of multi-paradigm models relying on different models of computation.

Model-based testing and simulation are complemented by runtime fault-tolerance through the automatic generation of software variants that can run in parallel, to tackle the open nature of software-intensive systems. The foundations in this case are the seminal work about N-version programming [67], recovery blocks [113] and code randomization [71], which demonstrated the central role of diversity in software to ensure runtime resilience of complex systems. Such techniques rely on truly diverse software solutions in order to provide systems with the ability to react to events, which could not be predicted at design time and checked through testing or simulation.

3.1.5. Empirical software engineering

The rigorous, scientific evaluation of DIVERSE's contributions is an essential aspect of our research methodology. In addition to theoretical validation through formal analysis or complexity estimation, we also aim at applying state-of-the-art methodologies and principles of empirical software engineering. This approach encompasses a set of techniques for the sound validation contributions in the field of software engineering,

[0] http://www.primordion.com/Xholon/

ranging from statistically sound comparisons of techniques and large-scale data analysis to interviews and systematic literature reviews [118], [116]. Such methods have been used for example to understand the impact of new software development paradigms [78]. Experimental design and statistical tests represent another major aspect of empirical software engineering. Addressing large-scale software engineering problems often requires the application of heuristics, and it is important to understand their effects through sound statistical analyses [66].

3.2. Research axis

Figure 1 illustrates the four dimensions of software diversity, which form the core research axis of DIVERSE: the **diversity of languages** used by the stakeholders involved in the construction of these systems; the **diversity of features** required by the different customers; the **diversity of runtime environments** in which software has to run and adapt; the **diversity of implementations** that are necessary for resilience through redundancy. These four axis share and leverage the scientific and technological results developed in the area of model-driven engineering in the last decade. This means that all our research activities are founded on sound abstractions to reason about specific aspects of software systems, compose different perspectives and automatically generate parts of the system.

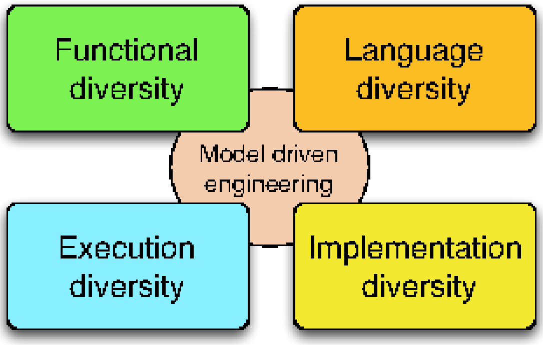


Figure 1. The four research axis of DIVERSE, which rely on a MDE scientific background

3.2.1. Software Language Engineering

The engineering of systems involves many different stakeholders, each with their own domain of expertise. Hence more and more organizations are adopting Domain Specific Modeling Languages (DSMLs) to allow domain experts to express solutions directly in terms of relevant domain concepts [117], [88]. This new trend raises new challenges about designing DSMLs, evolving a set of DSMLs and coordinating the use of multiple DSLs for both DSL designers and DSL users.

3.2.1.1. Challenges

Reusability of software artifacts is a central notion that has been thoroughly studied and used by both academics and industrials since the early days of software construction. Essentially, designing reusable artifacts allows the construction of large systems from smaller parts that have been separately developed and validated, thus reducing the development costs by capitalizing on previous engineering efforts. However, it is still hardly possible for language designers to design typical language artifacts (e.g. language constructs, grammars, editors or compilers) in a reusable way. The current state of the practice usually prevents the reusability of language artifacts from one language to another, consequently hindering the emergence of real engineering techniques around software languages. Conversely, concepts and mechanisms that enable artifacts reusability abound in the software engineering community.

Variability in modeling languages occur in the definition of the abstract and concrete syntax as well as in the specification of the language's semantics. The major challenges met when addressing the need for variability are: (i) set principles for modeling language units that support the modular specification of a modeling language; and (ii) design mechanisms to assemble these units in a complete language, according to the set of authorized variation points for the modeling language family.

A new generation of complex software-intensive systems (for example smart health support, smart grid, building energy management, and intelligent transportation systems) presents new opportunities for leveraging modeling languages. The development of these systems requires expertise in diverse domains. Consequently, different types of stakeholders (e.g., scientists, engineers and end-users) must work in a coordinated manner on various aspects of the system across multiple development phases. DSMLs can be used to support the work of domain experts who focus on a specific system aspect, but they can also provide the means for coordinating work across teams specializing in different aspects and across development phases. The support and integration of DSMLs leads to what we call **the globalization of modeling languages**, *i.e.* the use of multiple languages for the coordinated development of diverse aspects of a system. One can make an analogy with world globalization in which relationships are established between sovereign countries to regulate interactions (e.g., travel and commerce related interactions) while preserving each country's independent existence.

3.2.1.2. Scientific objectives

We address reuse and variability challenges through the investigation of the time-honored concepts of substitutability, inheritance and components, evaluate their relevance for language designers and provide tools and methods for their inclusion in software language engineering. We will develop novel techniques for the modular construction of language extensions with the support of model syntactical variability. From the semantics perspective, we investigate extension mechanisms for the specification of variability in operational semantics, focusing on static introduction and heterogeneous models of computation. The definition of variation points for the three aspects of the language definition provides the foundations for the novel concept Language Unit (LU) as well as suitable mechanisms to compose such units.

We explore the necessary breakthrough in software languages to support modeling and simulation of heterogeneous and open systems. This work relies on the specification of executable domain specific modeling languages (DSMLs) to formalize the various concerns of a software-intensive system, and of models of computation (MoCs) to explicitly model the concurrency, time and communication of such DSMLs. We develop a framework that integrates the necessary foundations and facilities for designing and implementing executable and concurrent domain-specific modeling languages. It also provides unique features to specify composition operators between (possibly heterogeneous) DSMLs. Such specifications are amenable to support the edition, execution, graphical animation and analysis of heterogeneous models. The objective is to provide both a significant improvement of MoCs and DSMLs design and implementation; and the simulation based validation and verification of complex systems.

We see an opportunity for the automatic diversification of programs' computation semantics, for example through the diversification of compilers or virtual machines. The main impact of this artificial diversity is to provide flexible computation and thus ease adaptation to different execution conditions. A combination of static and dynamic analysis could support the identification of what we call *plastic computation zones* in the code. We identify different categories of such zones: (i) areas in the code in which the order of computation can vary (e.g., the order in which a block of sequential statements is executed); (ii) areas that can be removed, keeping the essential functionality [119] (e.g., skip some loop iterations); (iii) areas that can replaced by alternative code (e.g., replace a try-catch by a return statement). Once we know which zones in the code can be randomized, it is necessary to modify the model of computation to leverage the computation plasticity. This consists in introducing variation points in the interpreter to reflect the diversity of models of computation. Then, the choice of a given variation is performed randomly at run-time.

3.2.2. Variability Modeling and Engineering

The systematic modeling of variability in software systems has emerged as an effective approach to document and reason about software evolutions and heterogeneity (*cf.* Section 3.1.2). Variability modeling characterizes an “envelope” of possible software variations. The industrial use of variability models and their relation to software artifact models require a complete engineering framework, including composition, decomposition, analysis, configuration and artifact derivation, refactoring, re-engineering, extraction, and testing. This framework can be used both to tame imposed diversity and to manage chosen diversity.

3.2.2.1. Challenges

A fundamental problem is that the **number of variants** can be exponential in the number of options (features). Already with 300 boolean configuration options, approximately 10^{90} configurations exist – more than estimated count of atoms in the universe. Domains like automotive or operating systems have to manage more than 10000 options (e.g., Linux). Practitioners face the challenge of developing billions of variants. It is easy to forget a necessary constraint, leading to the synthesis of unsafe variants, or to under-approximate the capabilities of the software platform. Scalable modelling techniques are therefore crucial to specify and reason about a very large set of variants.

Model-driven development supports two ways to deal with the increasing number of concerns in complex systems: (1) multi-view modeling, *i.e.* when modeling each concern separately, and variability modeling. However, there is little support to combine both approaches consistently. Techniques to integrate both approaches will enable the construction of a consistent set of views and variation points in each view.

The design, construction and maintenance of software families have a major impact on **software testing**. Among the existing challenges, we can cite: the selection of test cases for a specific variant; the evolution of test suites with integration of new variants; the combinatorial explosion of the number of software configurations to be tested. Novel model-based techniques for test generation and test management in a software product line context are needed to overcome state-of-the-art limits we already observed in some projects.

3.2.2.2. Scientific objectives

We aim at developing scalable techniques to automatically analyze variability models and their interactions with other views on the software intensive system (requirements, architecture, design). These techniques provide two major advancements in the state of the art: (1) an extension of the semantics of variability models in order to enable the definition of attributes (*e.g.*, cost, quality of service, effort) on features and to include these attributes in the reasoning; (2) an assessment of the consistent specification of variability models with respect to system views (since variability is orthogonal to system modeling, it is currently possible to specify the different models in ways that are semantically meaningless). The former aspect of analysis is tackled through constraint solving and finite-domain constraint programming, while the latter aspect is investigated through automatic search-based techniques (similar to genetic algorithms) for the exploration of the space of interaction between variability and view models.

We aim to develop procedures to reverse engineer dependencies and features’ sets from existing software artefacts – be it source code, configuration files, spreadsheets (e.g., product comparison matrices) or requirements. We expect to scale up (e.g., for extracting a very large number of variation points) and guarantee some properties (e.g., soundness of configuration semantics, understandability of ontological semantics). For instance, when building complex software-intensive systems, textual requirements are captured in very large quantities of documents. In this context, adequate models to formalize the organization of requirements documents and automated techniques to support impact analysis (in case of changes in the requirements) have to be developed.

We aim at developing sound methods and tools to integrate variability management in model-based testing activities. In particular, we will leverage requirement models as an essential asset to establish formal relations between variation points and test models. These relations will form the basis for novel algorithms that drive the systematic selection of test configurations that satisfy well-defined test adequacy criteria as well as the generation of test cases for a specific product in the product line.

3.2.3. Heterogeneous and dynamic software architectures

Flexible yet dependable systems have to cope with heterogeneous hardware execution platforms ranging from smart sensors to huge computation infrastructures and data centers. Evolutions range from a mere change in the system configuration to a major architectural redesign, for instance to support addition of new features or a change in the platform architecture (new hardware is made available, a running system switches to low bandwidth wireless communication, a computation node battery is running low, etc). In this context, we need to devise formalisms to reason about the impact of an evolution and about the transition from one configuration to another. It must be noted that this axis focuses on the use of models to drive the evolution from design time to run-time. Models will be used to (i) systematically define predictable configurations and variation points through which the system will evolve; (ii) develop behaviors necessary to handle unpredicted evolutions.

3.2.3.1. Challenges

The main challenge is to provide new homogeneous architectural modelling languages and efficient techniques that enable continuous software reconfiguration to react to changes. This work handles the challenges of handling the diversity of runtime infrastructures and managing the cooperation between different stakeholders. More specifically, the research developed in this axis targets the following dimensions of software diversity.

Platform architectural heterogeneity induces a first dimension of imposed diversity (type diversity). Platform reconfigurations driven by changing resources define another dimension of diversity (deployment diversity). To deal with these imposed diversity problems, we will rely on model based runtime support for adaptation, in the spirit of the dynamic distributed component framework developed by the Triskell team. Since the runtime environment composed of distributed, resource constrained hardware nodes cannot afford the overhead of traditional runtime adaptation techniques, we investigate the design of novel solutions relying on models@runtime and on specialized tiny virtual machines to offer resource provisioning and dynamic reconfigurations. In the next two years this research will be supported by the InfraJVM project.

Diversity can also be an asset to optimize software architecture. Architecture models must integrate multiple concerns in order to properly manage the deployment of software components over a physical platform. However, these concerns can contradict each other (*e.g.*, accuracy and energy). In this context, we investigate automatic solutions to explore the set of possible architecture models and to establish valid trade-offs between all concerns in case of changes.

3.2.3.2. Scientific objectives

Automatic synthesis of optimal software architectures. Implementing a service over a distributed platform (*e.g.*, a pervasive system or a cloud platform) consists in deploying multiple software components over distributed computation nodes. We aim at designing search-based solutions to (i) assist the software architect in establishing a good initial architecture (that balances between different factors such as cost of the nodes, latency, fault tolerance) and to automatically update the architecture when the environment or the system itself change. The choice of search-based techniques is motivated by the very large number of possible software deployment architectures that can be investigated and that all provide different trade-offs between qualitative factors. Another essential aspect that is supported by multi-objective search is to explore different architectural solutions that are not necessarily comparable. This is important when the qualitative factors are orthogonal to each other, such as security and usability for example.

Flexible software architecture for testing and data management. As the number of platforms on which software runs increases and different software versions coexist, the demand for testing environments also increases. For example, to test a software patch or upgrade, the number of testing environments is the product of the number of running environments the software supports and the number of coexisting versions of the software. Based on our first experiment on the synthesis of cloud environment using architectural models, our objective is to define a set of domain specific languages to catch the requirement and to design cloud environments for testing and data management of future internet systems from data centers to things. These languages will be interpreted to support dynamic synthesis and reconfiguration of a testing environment.

Runtime support for heterogeneous environments. Execution environments must provide a way to account or reserve resources for applications. However, current execution environments such as the Java Virtual Machine do not clearly define a notion of application: each framework has its own definition. For example, in OSGi, an application is a component, in JEE, an application is most of the time associated to a class loader, in the Multi-Tasking Virtual machine, an application is a process. The challenge consists in defining an execution environment that provides direct control over resources (CPU, Memory, Network I/O) independently from the definition of an application. We propose to define abstract resource containers to account and reserve resources on a distributed network of heterogeneous devices.

3.2.4. Diverse implementations for resilience

Open software-intensive systems have to evolve over their lifetime in response to changes in their environment. Yet, most verification techniques assume a closed environment or the ability to predict all changes. Dynamic changes and evolutions thus represent a major challenge for these techniques that aim at assessing the correctness and robustness of the system. On the one hand, DIVERSE will adapt V&V techniques to handle diversity imposed by the requirements and the execution environment, on the other hand we leverage diversity to increase the robustness of software in face of unpredicted situations. More specifically, we address the following V&V challenges.

3.2.4.1. Challenges

One major challenge to build flexible and open yet dependable systems is that current software engineering techniques require architects to foresee all possible situations the system will have to face. However, openness and flexibility also mean unpredictability: unpredictable bugs, attacks, environmental evolutions, etc. Current fault-tolerance [113] and security [87] techniques provide software systems with the capacity of detecting accidental and deliberate faults. However, existing solutions assume that the set of bugs or vulnerabilities in a system does not evolve. This assumption does not hold for open systems, thus it is essential to revisit fault-tolerance and security solutions to account for diverse and unpredictable faults.

Diversity is known to be a major asset for the robustness of large, open, and complex systems (*e.g.*, economical or ecological systems). Following this observation, the software engineering literature provides a rich set of work that choose to implement diversity in software systems in order to improve robustness to attacks or to changes in quality of service. These works range from N-version programming to obfuscation of data structures or control flow, to randomization of instruction sets. An essential remaining challenge is to support the automatic synthesis and evolution of software diversity in open software-intensive systems. There is an opportunity to further enhance these techniques in order to cope with a wider diversity of faults, by multiplying the levels of diversity in the different software layers that are found in software-intensive systems (system, libraries, frameworks, application). This increased diversity must be based on artificial program transformations and code synthesis, which increase the chances of exploring novel solutions, better fitted at one point in time. The biological analogy also indicates that diversity should emerge as a side-effect of evolution, to prevent over-specialization towards one kind of diversity.

3.2.4.2. Scientific objectives

The main objective is to address one of the main limitations of N-version programming for fault-tolerant systems: the manual production and management of software diversity. Through automated injection of artificial diversity we aim at systematically increasing failure diversity and thus increasing the chances of early error detection at run-time. A fundamental assumption for this work is that software-intensive systems can be “good enough” [114], [126].

Proactive program diversification. We aim at establishing novel principles and techniques that favor the emergence of multiple forms of software diversity in software-intensive systems, in conjunction with the software adaptation mechanisms that leverage this diversity. The main expected outcome is a set of meta-design principles that maintain diversity in systems and the experimental demonstration of the effects of software diversity on the adaptive capacities of CASs. Higher levels of diversity in the system provide a pool of software solutions that can eventually be used to adapt to situations unforeseen at design time (bugs, crash, attacks, etc.). Principles of automated software diversification rely on the automated synthesis of variants in a software product line, as well as finer-grained program synthesis combining unsound transformations and genetic programming to explore the space of mutational robustness.

Multi-tier software diversification. We call multi-tier diversification the fact of diversifying several application software components simultaneously. The novelty of our proposal, with respect to the software diversity state of the art, is to diversify the application-level code (for example, diversify the business logics of the application), focusing on the technical layers found in web applications. The diversification of application software code is expected to provide a diversity of failures and vulnerabilities in web server deployment. Web server deployment usually adopts a form of the Reactor architecture pattern, for scalability purposes: multiple copies of the server software stack, called request handlers, are deployed behind a load balancer. This architecture is very favorable for diversification, since by using the multiplicity of request handlers running in a web server we can simultaneously deploy multiple combinations of diverse software components. Then, if one handler is hacked or crashes the others should still be able to process client requests.

DYOGENE Project-Team

3. Research Program

3.1. Network Calculus

Network calculus [53] is a theory for obtaining deterministic upper bounds in networks that has been developed by R. Cruz [41], [42]. From the modelling point of view, it is an algebra for computing and propagating constraints given in terms of envelopes. A flow is represented by its cumulative function $R(t)$ (that is, the amount of data sent by the flow up to time t). A constraint on a flow is expressed by an arrival curve $\alpha(t)$ that gives an upper bound for the amount of data that can be sent during any interval of length t. Flows cross service elements that offer guarantees on the service. A constraint on a service is a service curve $\beta(t)$ that is used to compute the amount of data that can be served during an interval of length t. It is also possible to define in the same way minimal arrival curves and maximum service curves. Then such constraints envelop the processes and the services. Network calculus enables the following operations:

- computing the exact output cumulative function or at least bounding functions;
- computing output constraints for a flow (like an output arrival curve);
- computing the remaining service curve (that is, the service that of not used by the flows crossing a server);
- composing several servers in tandem;
- giving upper bounds on the worst-case delay and backlog (bounds are tight for a single server or a single flow).

The operations used for this are an adaptation of filtering theory to $(\min, +)$: $(\min, +)$ convolution and deconvolution, sub-additive closure.

We investigate the complexity of computing exact worst-case performance bounds in network calculus and to develop algorithms that present a good trade off between algorithmic efficiency and accuracy of the bounds.

3.2. Perfect Simulation

Simulation approaches can be used to efficiently estimate the stationary behavior of Markov chains by providing independent samples distributed according to their stationary distribution, even when it is impossible to compute this distribution numerically.

The classical Markov Chain Monte Carlo simulation techniques suffer from two main problems:

- The convergence to the stationary distribution can be very slow, and it is in general difficult to estimate;
- Even if one has an effective convergence criterion, the sample obtained after any finite number of iterations is biased.

To overcome these issues, Propp and Wilson [56] have introduced a perfect sampling algorithm (PSA) that has later been extended and applied in various contexts, including statistical physics [47], stochastic geometry [52], theoretical computer science [33], and communications networks [30], [46] (see also the bibliography at http://dimacs.rutgers.edu/~dbwilson/exact.html/ annotated by David B. Wilson.

Perfect sampling uses coupling arguments to give an unbiased sample from the stationary distribution of an ergodic Markov chain on a finite state space $\mathcal{X}$. Assume the chain is given by an update function Φ and an i.i.d. sequence of innovations $(U_n)_{n\in\mathbb{Z}}$, so that

$$X_{n+1} = \Phi(X_n, U_{n+1}). \tag{91}$$

The algorithm is based on a backward coupling scheme: it computes the trajectories from all $x \in \mathcal{X}$ at some time in the past $t = -T$ until time $t = 0$, using the same innovations. If the final state is the same for all trajectories (i.e. $|\{\Phi(x, U_{-T+1}, ..., U_0) : x \in \mathcal{X}\}| = 1$, where $\Phi(x, U_{-T+1}, ..., U_0) := \Phi(\Phi(x, U_{-T+1}), U_{-T+2}, ..., U_0)$ is defined by induction on T), then we say that the chain has globally coupled and the final state has the stationary distribution of the Markov chain. Otherwise, the simulations are started further in the past.

Any ergodic Markov chain on a finite state space has a representation of type (1) that couples in finite time with probability 1, so Propp and Wilson's PSA gives a "perfect" algorithm in the sense that it provides an *unbiased* sample in *finite time*. Furthermore, the stopping criterion is given by the coupling from the past scheme, and knowing the explicit bounds on the coupling time is not needed for the validity of the algorithm.

However, from the computational side, PSA is efficient only under some monotonicity assumptions that allow reducing the number of trajectories considered in the coupling from the past procedure only to extremal initial conditions. Our goal is to propose new algorithms solving this issue by exploiting semantic and geometric properties of the event space and the state space.

3.3. Stochastic Geometry

Stochastic geometry [40] is a rich branch of applied probability which allows one to quantify random phenomena on the plane or in higher dimension. It is intrinsically related to the theory of point processes. Initially its development was stimulated by applications to biology, astronomy and material sciences. Nowadays it is also widely used in image analysis. It provides a way of estimating and computing "spatial averages". A typical example, with obvious communication implications, is the so called Boolean model, which is defined as the union of discs with random radii (communication ranges) centered at the points of a Poisson point process (user locations) of the Euclidean plane (e.g., a city). A first typical question is that of the prediction of the fraction of the plane which is covered by this union (statistics of coverage). A second one is whether this union has an infinite component or not (connectivity). Further classical models include shot noise processes and random tessellations. Our research consists of analyzing these models with the aim of better understanding wireless communication networks in order to predict and control various network performance metrics. The models require using techniques from stochastic geometry and related fields including point processes, spatial statistics, geometric probability, percolation theory.

F. Baccelli, B. Blaszczyszyn in collaboration with M. Karray (Orange Labs) are preparing a new book focusing on the mathematical tools at the basis of stochastic geometry. The book will cover the main mathematical foundations of the field, namely the theory of point processes and random measures as well as the theory of random closed sets. The basis will be the graduate classes and the research courses taught by the authors at a variety of places worldwide.

The collaboration of F. Baccelli with V. Anantharam (UC Berkeley) continues in new directions on high dimensional stochastic geometry, primarily in relation with Information Theory, cf. Section 7.23 .

The collaboration of B. Blaszczyszyn with D. Yogeshwaran (Indian Statistical Institute) and Y. Yukich (Lehigh University) led to the development of the limit theory for geometric statistics on general input processes, cf. Section 7.22 .

3.4. Information Theory and Wireless Networks

Classical models of stochastic geometry (SG) are not sufficient for analyzing wireless networks as they ignore the specific nature of radio channels.

Consider a wireless communication network made of a collection of nodes which in turn can be transmitters or receivers. At a given time, some subset of this collection of nodes simultaneously transmit, each toward its own receiver. Each transmitter–receiver pair in this snapshot requires its own wireless link. For each such wireless link, the power of the signal received from the link transmitter is jammed by the powers of the signals received from the other transmitters. Even in the simplest model where the power radiated from a point decays in some isotropic way with Euclidean distance, the geometry of the location of nodes plays a key role within this setting since it determines the signal to interference and noise ratio (SINR) at the receiver of each such link and hence the possibility of establishing simultaneously this collection of links at a given bit rate, as shown by information theory (IT). In this definition, the interference seen by some receiver is the sum of the powers of the signals received from all transmitters excepting its own. The SINR field, which is of an essentially geometric nature, hence determines the connectivity and the capacity of the network in a broad sense. The essential point here is that the characteristics and even the feasibilities of the radio links that are simultaneously active are strongly interdependent and determined by the geometry. Our work is centered on the development of an IT-aware stochastic geometry addressing this interdependence. Dyogene members published in 2009 a two-volume book [1], [2] on Stochastic Geometry and Wireless Networks that became a reference publication in this domain.

In collaboration with Martin Haenggi (University of Notre Dame Notre Dame, IN, USA), Paul Keeler (Weierstrass Institute for Applied Analysis and Stochastics Berlin, Germany) and Sayandev Mukherjee (DOCOMO Innovations, Inc. Palo Alto, CA, USA), B. Blaszczyszyn is currently working on a book project that is intended to bridge a gap between academic and industrial approach to the design of next-generation cellular networks. In fact, simulation-only approach adopted by a majority of industry practitioners does not scale up with the increasing network complexity and analytical treatment is still yet not widely accepted in various bodies working out future standards specifications. The monograph is intended to bridge that gap, and make the methods, tools, approaches, and results of stochastic geometry available to a wide group of researchers (both in academia and in industry), systems engineers, and network designers. We expect that academic researchers and graduate students will appreciate that the book collects and organizes the most recent research results in a convenient way.

3.5. The Cavity Method for Network Algorithms

The cavity method combined with geometric networks concepts has recently led to spectacular progresses in digital communications through error-correcting codes. More than fifty years after Shannon's theorems, some coding schemes like turbo codes and low-density parity-check codes (LDPC) now approach the limits predicted by information theory. One of the main ingredients of these schemes is message-passing decoding strategies originally conceived by Gallager, which can be seen as direct applications of the cavity method on a random bipartite graph (with two types of nodes representing information symbols and parity check symbols, see [57]).

Modern coding theory is only one example of application of the cavity method. The concepts and techniques developed for its understanding have applications in theoretical computer science and a rich class of *complex systems*, in the field of networking, economics and social sciences. The cavity method can be used both for the analysis of randomized algorithms and for the study of random ensembles of computational problems representative real-world situations. In order to analyze the performance of algorithms, one generally defines a family of instances and endows it with a probability measure, in the same way as one defines a family of samples in the case of spin glasses or LDPC codes. The discovery that the hardest-to-solve instances, with all existing algorithms, lie close to a *phase transition* boundary has spurred a lot of interest. Theoretical physicists suggest that the reason is a structural one, namely a change in the geometry of the set of solutions related to the *replica symmetry breaking* in the cavity method. Phase transitions, which lie at the core of statistical physics, also play a key role in computer science [60], signal processing [44] and social sciences [49]. Their analysis is a major challenge, that may have a strong impact on the design of related algorithms.

We develop mathematical tools in the theory of discrete probabilities and theoretical computer science in order to contribute to a rigorous formalization of the cavity method, with applications to network algorithms, statistical inference, and at the interface between computer science and economics (EconCS).

3.6. Statistical Learning

Sparse graph structures are useful in a number of information processing tasks where the computational problem can be described as follows: infer the values of a large collection of random variables, given a set of constraints or observations, that induce relations among them. Similar design ideas have been proposed in sensing and signal processing and have applications in coding [38], network measurements, group testing or multi-user detection. While the computational problem is generally hard, sparse graphical structures lead to low-complexity algorithms that are very effective in practice. We develop tools in order to contribute to a precise analysis of these algorithms and of their gap to optimal inference which remains a largely open problem.

A second line of activities concerns the design of protocols and algorithms enabling a transmitter to learn its environment (the statistical properties of the channel quality to the corresponding receiver, as well as their interfering neighbouring transmitters) so as to optimise their transmission strategies and to fairly and efficiently share radio resources. This second objective calls for the development and use of machine learning techniques (e.g. bandit optimisation).

EVA Project-Team

3. Research Program

3.1. Generalities

EVA inherits its expertise in designing algorithms and protocols from HiPERCOM2 (e.g. OLSR). EVA also inherit know-how in modeling, simulation, experimentation and standardization. Through this know-how and experience, the results obtained are both far-reaching and useful.

3.2. Physical Layer

We plan to study how advanced physical layers can be used in low-power wireless networks. For instance, collaborative techniques such as multiple antennas (e.g. the Massive MIMO technology) can improve communication efficiency. The idea is to use a massive network densification by drastically increasing the number of sensors in a given area in a Time Division Duplex (TDD) mode with time reversal. The first period allows the sensors to estimate the channel state and, after time reversal, the second period is to transmit the data sensed. Other techniques, such as interference cancellation, are also possible.

3.3. Wireless Access

Medium sharing in wireless systems has received substantial attention throughout the last decade. HiPERCOM2 has provided models to compare TDMA and CSMA. HiPERCOM2 has also studied how network nodes must be positioned to optimize the global throughput.

EVA will pursue modeling tasks to compare access protocols, including multi-carrier access, adaptive CSMA (particularly in VANETs), as well as directional and multiple antennas. There is a strong need for determinism in industrial networks. The EVA team will focus particularly on scheduled medium access in the context of deterministic industrial networks; this will involve optimizing the joint time slot and channel assignment. Distributed approaches will be considered, and the EVA team will determine their limits in terms of reliability, latency and throughput. Furthermore, adaptivity to application or environment changes will be taken into account.

3.4. Coexistence of Wireless Technologies

Wireless technologies such as cellular, low-power mesh networks, (Low-Power) WiFi, and Bluetooth (low-energy) can reasonably claim to fit the requirements of the IoT. Each, however, uses different trade-offs between reliability, energy consumption and throughput. The EVA team will study the limits of each technology, and will develop clear criteria to evaluate which technology is best suited to a particular set of constraints.

Coexistence between these different technologies (or different deployments of the same technology in a common radio space) is a valid point of concern.

The EVA team aims at studying such coexistence, and, where necessary, propose techniques to improve it. Where applicable, the techniques will be put forward for standardization. Multiple technologies can also function in a symbiotic way.

For example, to improve the quality of experience provided to end users, a wireless mesh network can transport sensor and actuator data in place of a cellular network, when and where cellular connectivity is poor.

The EVA team will study how and when different technologies can complement one another. A specific example of a collaborative approach is Cognitive Radio Sensor Networks (CRSN).

3.5. Energy-Efficiency and Determinism

Reducing the energy consumption of low-power wireless devices remains a challenging task. The overall energy budget of a system can be reduced by using less power-hungry chips, and significant research is being done in that direction. Nevertheless, power consumption is mostly influenced by the algorithms and protocols used in low-power wireless devices, since they influence the duty-cycle of the radio.

EVA will search for energy-efficient mechanisms in low-power wireless networks. One new requirement concerns the ability to predict energy consumption with a high degree of accuracy. Scheduled communication, such as the one used in the IEEE 802.15.4e TSCH (Time Slotted CHannel Hopping) standard, and by IETF 6TiSCH, allows for a very accurate prediction of the energy consumption of a chip. Power conservation will be a key issue in EVA.

To tackle this issue and match link-layer resources to application needs, EVA's 5-year research program around Energy-Efficiency and Determinism centers around 3 studies:

- Performance Bounds of a TSCH network. We propose to study a low-power wireless TSCH network as a Networked Control System (NCS), and use results from the NCS literature. A large number of publications on NCS, although dealing with wireless systems, consider wireless links to have perfect reliability, and do not consider packet loss. Results from these papers can not therefore be applied directly to TSCH networks. Instead of following a purely mathematical approach to model the network, we propose to use a non-conventional approach and build an empirical model of a TSCH network.
- Distributed Scheduling in TSCH networks. Distributed scheduling is attractive due to its scalability and reactivity, but might result in a sub-optimal schedule. We continue this research by designing a distributed solution based on control theory, and verify how this solution can satisfy service level agreements in a dynamic environment.

3.6. Network Deployment

Since sensor networks are very often built to monitor geographical areas, sensor deployment is a key issue. The deployment of the network must ensure full/partial, permanent/intermittent coverage and connectivity. This technical issue leads to geometrical problems which are unusual in the networking domain.

We can identify two scenarios. In the first one, sensors are deployed over a given area to guarantee full coverage and connectivity, while minimizing the number of sensor nodes. In the second one, a network is re-deployed to improve its performance, possibly by increasing the number of points of interest covered, and by ensuring connectivity. EVA will investigate these two scenarios, as well as centralized and distributed approaches. The work starts with simple 2D models and will be enriched to take into account more realistic environment: obstacles, walls, 3D, fading.

3.7. Data Gathering and Dissemination

A large number of WSN applications mostly do data gathering (a.k.a "convergecast"). These applications usually require small delays for the data to reach the gateway node, requiring time consistency across gathered data. This time consistency is usually achieved by a short gathering period.

In many real WSN deployments, the channel used by the WSN usually encounters perturbations such as jamming, external interferences or noise caused by external sources (e.g. a polluting source such as a radar) or other coexisting wireless networks (e.g. WiFi, Bluetooth). Commercial sensor nodes can communicate on multiple frequencies as specified in the IEEE 802.15.4 standard. This reality has given birth to the multichannel communication paradigm in WSNs.

Multichannel WSNs significantly expand the capability of single-channel WSNs by allowing parallel transmissions, and avoiding congestion on channels or performance degradation caused by interfering devices.

In EVA, we will focus on raw data convergecast in multichannel low-power wireless networks. In this context, we are interested in centralized/distributed algorithms that jointly optimize the channel and time slot assignment used in a data gathering frame. The limits in terms of reliability, latency and bandwidth will be evaluated. Adaptivity to additional traffic demands will be improved.

3.8. Self-Learning Networks

To adapt to varying conditions in the environment and application requirements, the EVA team will investigate self-learning networks. Machine learning approaches, based on experts and forecasters, will be investigated to predict the quality of the wireless links in a WSN. This allows the routing protocol to avoid using links exhibiting poor quality and to change the route before a link failure. Additional applications include where to place the aggregation function in data gathering. In a content delivery network (CDN), it is very useful to predict the popularity, expressed by the number of solicitations per day, of a multimedia content. The most popular contents are cached near the end-users to maximize the hit ratio of end-users' requests. Thus the satisfaction degree of end-users is maximized and the network overhead is minimized.

3.9. Security Trade-off in Constrained Wireless Networks

Ensuring security is a sine qua non condition for the widespread acceptance and adoption of the IoT, in particular in industrial and military applications. While the Public-Key Infrastructure (PKI) approach is ubiquitous on the traditional Internet, constraints in terms of embedded memory, communication bandwidth and computational power make translating PKI to constrained networks non-trivial.

Two related standardization working groups were created in 2013 to address this issue. DICE (DTLS In Constrained Environments) is defining a DTLS (Datagram Transport Layer Security) profile that is suitable for IoT applications, using the (Constrained Application Protocol) CoAP protocol. ACE is standardizing authentication and authorization mechanisms for constrained environments.

The issue is to find the best trade-off between a communication and computation overhead compatible with the limited capacity of sensor nodes and the level of protection required by the application.

FOCUS Project-Team

3. Research Program

3.1. Models

The objective of Focus is to develop concepts, techniques, and possibly also tools, that may contribute to the analysis and synthesis of CBUS. Fundamental to these activities is *modeling*. Therefore designing, developing and studying computational models appropriate for CBUS is a central activity of the project. The models are used to formalise and verify important computational properties of the systems, as well as to propose new linguistic constructs.

The models we study are in the process calculi (e.g., the π-calculus) and λ-calculus tradition. Such models, with their emphasis on algebra, well address compositionality—a central property in our approach to problems. Accordingly, the techniques we employ are mainly operational techniques based on notions of behavioural equivalence, and techniques based on algebra, mathematical logics, and type theory.

FUN Project-Team

3. Research Program

3.1. Introduction

We will focus on wireless ubiquitous networks that rely on constrained devices, i.e. with limited resources in terms of storage and computing capacities. They can be sensors, small robots, RFID readers or tags. A wireless sensor retrieves a physical measure such as light. A wireless robot is a wireless sensor that in addition has the ability to move by itself in a controlled way. A drone is a robot with the ability to manoeuvre in 3D (in the air or in the water). RFID tags are passive items that embed a unique identifier for a place or an object allowing accurate traceability. They can communicate only in the vicinity of an RFID reader. An RFID reader can be seen as a special kind of sensor in the network which data is the one read on tags. These devices may run on batteries that are not envisaged to be changed or recharged. These networks may be composed of ten to thousands of such heterogeneous devices for which energy is a key issue.

Today, most of these networks are homogeneous, i.e. composed of only one kind of devices. They have mainly been studied in application and technology silos. Because of this, they are approaching fundamental limitations especially in terms of topology deployment, management and communications, while exploiting the complementarity of heterogeneous devices and communication technologies would enlarge their capacities and the set of applications. Finally, these networks must work efficiently even in dynamic and realistic situations, i.e. they must consider by design the different dynamic parameters and automatically self-adapt to their variations.

Our overall goal is represented by Figure 1 . We will investigate wireless ubiquitous IoT services for constrained devices by smartly combining **different frequency bands** and **different medium access and routing techniques**over **heterogeneous devices** in a **distributed** and **opportunistic** fashion. Our approach will always deal with **hardware constraints** and take care of **security** and **energy** issues to provide protocols that ride on **synergy** and **self-organization** between devices.

The goal of the FUN project team is to provide these next generation networks with a set of innovative and distributed self-organizing cooperative protocols to raise them to a new level of scalability, autonomy, adaptability, manageability and performance. We aim to break these silos to exploit the full synergy between devices, making them cooperate in a single holistic network. We will consider them as networks of heterogeneous devices rather than a collection of heterogeneous networks.

To realize the full potential of these ubiquitous networks, there is a need to provide them with a set of tools that allow them to *(i)* (self-)deploy, *(ii)* self-organize, *(iii)* discover and locate each other, resources and services and *(iv)* communicate. These tools will be the basics for enabling cooperation, co-existence and witnessing a global efficient behavior. The deployment of these mechanisms is challenging since it should be achieved in spite of several limitations. The main difficulties are to provide such protocols in a **secured** and **energy-efficient** fashion in spite of :

- dynamic topology changes due to various factors such as the unreliability of the wireless medium, the wireless interferences between devices, node mobility and energy saving mechanisms;
- hardware constraints in terms of CPU and memory capacities that limit the operations and data each node can perform/collect;
- lacks of interoperability between applicative, hardware and technological silos that may prevent from data exchange between different devices.

3.1.1. Objectives and methodology

To reach our overall goal, we will pursue the two following objectives, similar to the ones we set for the previous evaluation period. These two objectives are othogonal and can be carried on jointly :

1. Providing realistic complete self-organizing tools *e.g. vertical perspective*.
2. Going to heterogeneous energy-efficient performing wireless networks *e.g. horizontal perspective*,

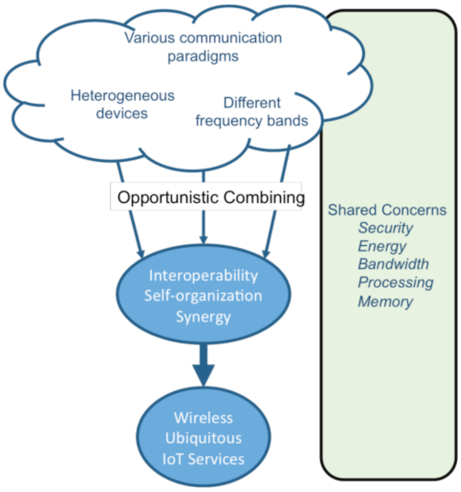


Figure 1. FUN’s overal goal.

We give more details on these two objectives below. To achieve our main objectives, we will mainly apply the methodology depicted in Figure 2 combining both theoretical analysis and experimental validation. Mathematical tools will allow us to properly dimension a problem, formally define its limitations and needs to provide suitable protocols in response. Then, they will allow us to qualify the outcome solutions before we validate and stress them in real scenarios with regards to applications requirements. For this, we will realize proofs-of-concept with real scenarios and real devices. Differences between results and expectations will be analyzed in return in order to well understand them and integrate them by design for a better protocol self-adaptation capability.

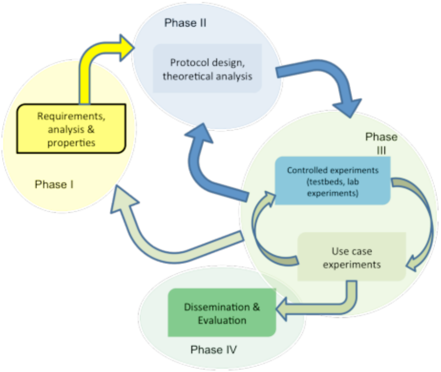

Phase II
Protocol design, theoretical analysis
Requirements, analysis & properties
Phase I
Phase III
Controlled experiments (testbeds, lab experiments)
Use case experiments
Dissemination & Evaluation
Phase IV

Figure 2. Methodology to be applied in FUN.

3.2. Vertical Perspective

As mentioned, future ubiquitous networks evolve in dynamic and unpredictable environments. Also, they can be used in a large scope of applications that have several expectations in terms of performance and different contextual limitations. In this heterogeneous context, IoT devices must support multiple applications and relay traffic with non-deterministic pattern.

To make our solutions practical and efficient in real conditions, we will adopt the dual approach both *top-down* and *bottom-up*. The *top-down* approach will ensure that we consider the application (such as throughput, delay, energy consumption, etc) and environmental limitations (such as deployment constraints, etc). The *bottom-up* approach will ensure that we take account of the physical and hardware characteristics such as memory, CPU, energy capacities but also physical interferences and obstacles. With this integrated perpective, we will be in capacity to design **cross-layer** integrated protocols well adapted [39]. We will design jointly routing and MAC layers by taking dynamics occurring at the physical layer into account with a constant concern for energy and security. We will investigate new adaptive frequency hopping techniques combined with routing protocols [41], [50], [24]. Also, we will work on new scheduling techniques for TSCH (a MAC layer of IEEE 802.15.4e) that are able work under the above-mentionned assumptions and bring the robustness of TSCH to IoT scenarios. We will investigate the performance boundaries of TSCH in particular in terms of energy-efficiency of time synchronization [63], and will propose alternative approaches such as capture effect-based time synchronization in TSCH or opportunistic routing. Another technology we will consider is IEEE 802.15.4g, which provides communication ranges in the order of tens of kilometers. We will propose mechanisms to support scaling up to networks with a density of hundreds of nodes, at the MAC layer and above. We will also consider dual-technology networks where both long and short-range communication cooperate for increased robustness.

This vision will also allow us to integrate external factors by design in our protocols, in an opportunistic way. Yet, we will leverage on the occurrence of any of these phenomena rather than perceiving them as obstacles or limitations. As an example, we will rely on node undergone mobility to enhance routing performance as we have started to investigate in [74], [59]. On the same idea, when specific features are available like controlled mobility, we will exploit it to improve connectivity or coverage quality like in [46] [67].

3.3. Horizontal perspective

We aim at designing efficient tools for a plethora of wireless devices supporting highly heterogeneous technologies. We will thus investigate these networks from a horizontal perspective, e.g. by considering heterogeneity in low level communications layers.

Given the spectrum scarcity, they will probably need to coexist in the same frequency bands and sometimes for different purposes (RFID tag reading may use the same frequency bands as the wireless sensors). One important aspect to consider in this setting is how these different access technologies will interact with each other and what are the mechanisms needed to be put in place to guarantee that all services obtain the required share of resources when needed. This problem appears in different application domains, ranging from traffic offloading to unlicensed bands by cellular networks and the need to coexist with WiFi and radars, from a scenario in which multiple-purpose IoT clouds coexist in a city [75]. We will thus explore the dynamics of these interactions and devise ways to ensure smooth coexistence while considering the heterogeneity of the devices involved, the access mechanisms used as well as the requirements of the services provided.

To face the spectrum scarcity, we will also investigate new alternative communication paradigms such as phonon-based or light-based communications as we have initiated in [70], [71][16] and we will work on the coexistence of these technologies with traditional communication techniques, specifically by investigating efficient switching techniques from one communication technology to the other (they were most focused on the security aspects, to prevent jamming attacks). Resilience and reliability of the whole system will be the key factors to be taken into account [50], [24].

As a more prospective activity, we consider exploring software and communication security for IoT. This is challenging given that existing solutions do not address systems that are both constrained and networked [63]. Finally, in order to contribute to a better interoperability between all these technologies, we will continue to contribute to standardization bodies such as IETF and EPC Global.

GANG Project-Team

3. Research Program

3.1. Graph and Combinatorial Algorithms

We focus on two approaches for designing algorithms for large graphs: decomposing the graph and relying on simple graph traversals.

3.1.1. Graph Decompositions

We study new decompositions schemes such as 2-join, skew partitions and others partition problems. These graph decompositions appeared in the structural graph theory and are the basis of some well-known theorems such as the Perfect Graph Theorem. For these decompositions there is a lack of efficient algorithms. We aim at designing algorithms working in $O(nm)$ since we think that this could be a lower bound for these decompositions.

3.1.2. Graph Search

We more deeply study multi-sweep graph searches. In this domain a graph search only yields a total ordering of the vertices which can be used by the subsequent graph searches. This technique can be used on huge graphs and do not need extra memory. We already have obtained preliminary results in this direction and many well-known graph algorithms can be put in this framework. The idea behind this approach is that each sweep discovers some structure of the graph. At the end of the process either we have found the underlying structure (for example an interval representation for an interval graph) or an approximation of it (for example in hard discrete optimization problems). We envision applications to exact computations of centers in huge graphs, to underlying combinatorial optimization problems, but also to networks arising in biology.

3.1.3. Graph Exploration

In the course of graph exploration, a mobile agent is expected to regularly visit all the nodes of an unknown network, trying to discover all its nodes as quickly as possible. Our research focuses on the design and analysis of agent-based algorithms for exploration-type problems, which operate efficiently in a dynamic network environment, and satisfy imposed constraints on local computational resources, performance, and resilience. Our recent contributions in this area concern the design of fast deterministic algorithms for teams of agents operating in parallel in a graph, with limited or no persistent state information available at nodes. We plan further studies to better understand the impact of memory constraints and of the availability of true randomness on efficiency of the graph exploration process.

3.2. Distributed Computing

The distributed community can be viewed as the union of two sub-communities. This is true even in our team. Even though they are not completely disjoint, they are disjoint enough not to leverage each others' results. At a high level, one is mostly interested in timing issues (clock drifts, link delays, crashes, etc.) while the other one is mostly interested in spatial issues (network structure, memory requirements, etc.). Indeed, one sub-community is mostly focusing on the combined impact of asynchronism and faults on distributed computation, while the other addresses the impact of network structural properties on distributed computation. Both communities address various forms of computational complexities, through the analysis of different concepts. This includes, e.g., failure detectors and wait-free hierarchy for the former community, and compact labeling schemes and computing with advice for the latter community. We have the ambitious project to achieve the reconciliation between the two communities by focusing on the same class of problems, the yes/no-problems, and establishing the scientific foundations for building up a consistent theory of computability and complexity for distributed computing. The main question addressed is therefore: is the absence of globally coherent computational complexity theories covering more than fragments of distributed computing, inherent to the field? One issue is obviously the types of problems located at the core of distributed computing. Tasks like consensus, leader election, and broadcasting are of very different nature. They are not *yes-no* problems, neither are they minimization problems. Coloring and Minimal Spanning Tree are optimization problems but we are often more interested in constructing an optimal solution than in verifying the correctness of a given solution. Still, it makes full sense to analyze the *yes-no* problems corresponding to checking the validity of the output of tasks. Another issue is the power of individual computation. The FLP impossibility result as well as Linial's lower bound hold independently from the individual computational power of the involved computing entities. For instance, the individual power of solving NP-hard problems in constant time would not help overcoming these limits which are inherent to the fact that computation is distributed. A third issue is the abundance of models for distributed computing frameworks, from shared memory to message passing, spanning all kinds of specific network structures (complete graphs, unit-disk graphs, etc.) and or timing constraints (from complete synchronism to full asynchronism). There are however models, typically the wait-free model and the LOCAL model, which, though they do not claim to reflect accurately real distributed computing systems, enable focusing on some core issues. Our research program is ongoing to carry many important notions of Distributed Computing into a *standard* computational complexity.

3.3. Network Algorithms and Analysis

Based on our scientific foundation on both graph algorithms and distributed algorithms, we plan to analyze the behavior of various networks such as future Internet, social networks, overlay networks resulting from distributed applications or online social networks.

3.3.1. Information Dissemination

One of the key aspects of networks resides in the dissemination of information among the nodes. We aim at analyzing various procedures of information propagation from dedicated algorithms to simple distributed schemes such as flooding. We also consider various models, where noise can alter information as it propagates or where memory of nodes is limited for example.

3.3.2. Routing Paradigms

We try to explore new routing paradigms such as greedy routing in social networks for example. We are also interested in content centric networking where routing is based on content name rather than content address. One of our target is multiple path routing: how to design forwarding tables providing multiple disjoint paths to a destination?

3.3.3. Beyond Peer-to-Peer

Based on our past experience of peer-to-peer application design, we would like to broaden the spectrum of distributed applications where new efficient algorithms and analysis can be performed. We especially target online social networks if we see them as collaborative tools for exchanging information. A basic question resides in making the right connections for gathering filtered and accurate information with sufficient coverage.

3.3.4. SAT and Forwarding Information Verification

As forwarding tables of networks grow and are sometimes manually modified, the problem of verifying forwarding information becomes critical and has recently gained in interest. Some problems that arise in network verification such as loop detection for example, may be naturally encoded as Boolean Satisfiability problems. Beside the theoretical interest of this encoding in complexity proofs, it has also a practical value for solving these problems by taking advantage of the many efficient Satisfiability testing solvers. Indeed, SAT solvers have proved to be very efficient in solving problems coming from various areas (Circuit Verification, Dependency and Conflicts in Software distributions...) and encoded in Conjunctive Normal Form. To test an approach using SAT solvers in network verification, one need to collect data sets from real network and to develop good models for generating realistic networks. The technique of encoding and the solvers themselves need to be adapted to this kind of problems. All this represent a rich experimental field of future research.

3.3.5. Network Analysis

Finally, we are interested in analyzing the structural properties of practical networks. This can include diameter computation or ranking of nodes. As we mostly consider large networks, we are often interested in efficient heuristics. Ideally, we target heuristics that give exact answer although fast computation time is not guaranteed for all networks. We already have designed such heuristics for diameter computation; understanding the structural properties that enable fast computation time in practice is still an open question.

HIEPACS Project-Team

3. Research Program

3.1. Introduction

The methodological component of HIEPACS concerns the expertise for the design as well as the efficient and scalable implementation of highly parallel numerical algorithms to perform frontier simulations. In order to address these computational challenges a hierarchical organization of the research is considered. In this bottom-up approach, we first consider in Section 3.2 generic topics concerning high performance computational science. The activities described in this section are transversal to the overall project and their outcome will support all the other research activities at various levels in order to ensure the parallel scalability of the algorithms. The aim of this activity is not to study general purpose solution but rather to address these problems in close relation with specialists of the field in order to adapt and tune advanced approaches in our algorithmic designs. The next activity, described in Section 3.3 , is related to the study of parallel linear algebra techniques that currently appear as promising approaches to tackle huge problems on extreme scale platforms. We highlight the linear problems (linear systems or eigenproblems) because they are in many large scale applications the main computational intensive numerical kernels and often the main performance bottleneck. These parallel numerical techniques, which are involved in the IPL C2S@EXA, will be the basis of both academic and industrial collaborations, some are described in Section 4.1 , but will also be closely related to some functionalities developed in the parallel fast multipole activity described in Section 3.4 . Finally, as the accuracy of the physical models increases, there is a real need to go for parallel efficient algorithm implementation for multiphysics and multiscale modeling in particular in the context of code coupling. The challenges associated with this activity will be addressed in the framework of the activity described in Section 3.5 .

Currently, we have one major application (see Section 4.1) that is in material physics. We will collaborate to all steps of the design of the parallel simulation tool. More precisely, our applied mathematics skill will contribute to the modelling, our advanced numerical schemes will help in the design and efficient software implementation for very large parallel simulations. We also participate to a few co-design actions in close collaboration with some applicative groups, some of them being involved in the IPL C2S@EXA. The objective of this activity is to instantiate our expertise in fields where they are critical for designing scalable simulation tools. We refer to Section 4.2 for a detailed description of these activities.

3.2. High-performance computing on next generation architectures

Participants: Emmanuel Agullo, Olivier Coulaud, Mathieu Faverge, Luc Giraud, Abdou Guermouche, Matias Hastaran, Guillaume Latu, Grégoire Pichon, Florent Pruvost, Pierre Ramet, Jean Roman, Emrullah Fatih Yetkin.

The research directions proposed in HIEPACS are strongly influenced by both the applications we are studying and the architectures that we target (i.e., massively parallel heterogeneous many-core architectures, ...). Our main goal is to study the methodology needed to efficiently exploit the new generation of high-performance computers with all the constraints that it induces. To achieve this high-performance with complex applications we have to study both algorithmic problems and the impact of the architectures on the algorithm design.

From the application point of view, the project will be interested in multiresolution, multiscale and hierarchical approaches which lead to multi-level parallelism schemes. This hierarchical parallelism approach is necessary to achieve good performance and high-scalability on modern massively parallel platforms. In this context, more specific algorithmic problems are very important to obtain high performance. Indeed, the kind of applications we are interested in are often based on data redistribution for example (e.g., code coupling applications). This well-known issue becomes very challenging with the increase of both the number of computational nodes and the amount of data. Thus, we have both to study new algorithms and to adapt the existing ones. In addition, some issues like task scheduling have to be restudied in this new context. It is important to note that the work developed in this area will be applied for example in the context of code coupling (see Section 3.5).

Considering the complexity of modern architectures like massively parallel architectures or new generation heterogeneous multicore architectures, task scheduling becomes a challenging problem which is central to obtain a high efficiency. Of course, this work requires the use/design of scheduling algorithms and models specifically to tackle our target problems. This has to be done in collaboration with our colleagues from the scheduling community like for example O. Beaumont (Inria REALOPT Project-Team). It is important to note that this topic is strongly linked to the underlying programming model. Indeed, considering multicore architectures, it has appeared, in the last five years, that the best programming model is an approach mixing multi-threading within computational nodes and message passing between them. In the last five years, a lot of work has been developed in the high-performance computing community to understand what is critic to efficiently exploit massively multicore platforms that will appear in the near future. It appeared that the key for the performance is firstly the granularity of the computations. Indeed, in such platforms the granularity of the parallelism must be small so that we can feed all the computing units with a sufficient amount of work. It is thus very crucial for us to design new high performance tools for scientific computing in this new context. This will be developed in the context of our solvers, for example, to adapt to this new parallel scheme. Secondly, the larger the number of cores inside a node, the more complex the memory hierarchy. This remark impacts the behaviour of the algorithms within the node. Indeed, on this kind of platforms, NUMA effects will be more and more problematic. Thus, it is very important to study and design data-aware algorithms which take into account the affinity between computational threads and the data they access. This is particularly important in the context of our high-performance tools. Note that this work has to be based on an intelligent cooperative underlying run-time (like the tools developed by the Inria STORM Project-Team) which allows a fine management of data distribution within a node.

Another very important issue concerns high-performance computing using "heterogeneous" resources within a computational node. Indeed, with the deployment of the GPU and the use of more specific co-processors, it is important for our algorithms to efficiently exploit these new type of architectures. To adapt our algorithms and tools to these accelerators, we need to identify what can be done on the GPU for example and what cannot. Note that recent results in the field have shown the interest of using both regular cores and GPU to perform computations. Note also that in opposition to the case of the parallelism granularity needed by regular multicore architectures, GPU requires coarser grain parallelism. Thus, making both GPU and regular cores work all together will lead to two types of tasks in terms of granularity. This represents a challenging problem especially in terms of scheduling. From this perspective, we investigate new approaches for composing parallel applications within a runtime system for heterogeneous platforms.

In that framework, the SOLHAR project aims at studying and designing algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computers equipped with accelerators. Several attempts have been made to accomplish the porting of these methods on such architectures; the proposed approaches are mostly based on a simple offloading of some computational tasks (the coarsest grained ones) to the accelerators and rely on fine hand-tuning of the code and accurate performance modeling to achieve efficiency. SOLHAR proposes an innovative approach which relies on the efficiency and portability of runtime systems, such as the StarPU tool developed in the STORM team. Although the SOLHAR project will focus on heterogeneous computers equipped with GPUs due to their wide availability and affordable cost, the research accomplished on algorithms, methods and programming models will be readily applicable to other accelerator devices. Our final goal would be to have high performance solvers and tools which can efficiently run on all these types of complex architectures by exploiting all the resources of the platform (even if they are heterogeneous).

In order to achieve an advanced knowledge concerning the design of efficient computational kernels to be used on our high performance algorithms and codes, we will develop research activities first on regular frameworks before extending them to more irregular and complex situations. In particular, we will work first on optimized dense linear algebra kernels and we will use them in our more complicated direct and hybrid solvers for sparse linear algebra and in our fast multipole algorithms for interaction computations. In this context, we will participate to the development of those kernels in collaboration with groups specialized in dense linear algebra. In particular, we intend develop a strong collaboration with the group of Jack Dongarra at the University of Tennessee and collaborating research groups. The objectives will be to develop dense linear algebra algorithms and libraries for multicore architectures in the context the PLASMA project and for GPU and hybrid multicore/GPU architectures in the context of the MAGMA project. The framework that hosts all these research activities is the associate team MORSE. A new solver has emerged from the associate team, Chameleon. While PLASMA and MAGMA focus on multicore and GPU architectures, respectively, Chameleon makes the most out of heterogeneous architectures thanks to task-based dynamic runtime systems.

A more prospective objective is to study the resiliency in the context of large-scale scientific applications for massively parallel architectures. Indeed, with the increase of the number of computational cores per node, the probability of a hardware crash on a core or of a memory corruption is dramatically increased. This represents a crucial problem that needs to be addressed. However, we will only study it at the algorithmic/application level even if it needed lower-level mechanisms (at OS level or even hardware level). Of course, this work can be performed at lower levels (at operating system) level for example but we do believe that handling faults at the application level provides more knowledge about what has to be done (at application level we know what is critical and what is not). The approach that we will follow will be based on the use of a combination of fault-tolerant implementations of the run-time environments we use (like for example ULFM) and an adaptation of our algorithms to try to manage this kind of faults. This topic represents a very long range objective which needs to be addressed to guaranty the robustness of our solvers and applications. In that respect, we are involved in the EXA2CT FP7 project.

Finally, it is important to note that the main goal of HIEPACS is to design tools and algorithms that will be used within complex simulation frameworks on next-generation parallel machines. Thus, we intend with our partners to use the proposed approach in complex scientific codes and to validate them within very large scale simulations as well as designing parallel solution in co-design collaborations.

3.3. High performance solvers for large linear algebra problems

Participants: Emmanuel Agullo, Olivier Coulaud, Mathieu Faverge, Aurélien Falco, Luc Giraud, Abdou Guermouche, Yuval Harness, Matias Hastaran, Matthieu Kuhn, Gilles Marait, Julien Pedron, Cyrille Piacibello, Grégoire Pichon, Louis Poirel, Pierre Ramet, Jean Roman.

Starting with the developments of basic linear algebra kernels tuned for various classes of computers, a significant knowledge on the basic concepts for implementations on high-performance scientific computers has been accumulated. Further knowledge has been acquired through the design of more sophisticated linear algebra algorithms fully exploiting those basic intensive computational kernels. In that context, we still look at the development of new computing platforms and their associated programming tools. This enables us to identify the possible bottlenecks of new computer architectures (memory path, various level of caches, inter processor or node network) and to propose ways to overcome them in algorithmic design. With the goal of designing efficient scalable linear algebra solvers for large scale applications, various tracks will be followed in order to investigate different complementary approaches. Sparse direct solvers have been for years the methods of choice for solving linear systems of equations, it is nowadays admitted that classical approaches are not scalable neither from a computational complexity nor from a memory view point for large problems such as those arising from the discretization of large 3D PDE problems. We will continue to work on sparse direct solvers on the one hand to make sure they fully benefit from most advanced computing platforms and on the other hand to attempt to reduce their memory and computational costs for some classes of problems where data sparse ideas can be considered. Furthermore, sparse direct solvers are a key building boxes for the design of some of our parallel algorithms such as the hybrid solvers described in the sequel of this section. Our activities in that context will mainly address preconditioned Krylov subspace methods; both components, preconditioner and Krylov solvers, will be investigated. In this framework, and possibly in relation with the research activity on fast multipole, we intend to study how emerging $\mathcal{H}$-matrix arithmetic can benefit to our solver research efforts.

3.3.1. Parallel sparse direct solver

For the solution of large sparse linear systems, we design numerical schemes and software packages for direct and hybrid parallel solvers. Sparse direct solvers are mandatory when the linear system is very ill-conditioned; such a situation is often encountered in structural mechanics codes, for example. Therefore, to obtain an industrial software tool that must be robust and versatile, high-performance sparse direct solvers are mandatory, and parallelism is then necessary for reasons of memory capability and acceptable solution time. Moreover, in order to solve efficiently 3D problems with more than 50 million unknowns, which is now a reachable challenge with new multicore supercomputers, we must achieve good scalability in time and control memory overhead. Solving a sparse linear system by a direct method is generally a highly irregular problem that induces some challenging algorithmic problems and requires a sophisticated implementation scheme in order to fully exploit the capabilities of modern supercomputers.

New supercomputers incorporate many microprocessors which are composed of one or many computational cores. These new architectures induce strongly hierarchical topologies. These are called NUMA architectures. In the context of distributed NUMA architectures, in collaboration with the Inria STORM team, we study optimization strategies to improve the scheduling of communications, threads and I/O. We have developed dynamic scheduling designed for NUMA architectures in the PaStiX solver. The data structures of the solver, as well as the patterns of communication have been modified to meet the needs of these architectures and dynamic scheduling. We are also interested in the dynamic adaptation of the computation grain to use efficiently multi-core architectures and shared memory. Experiments on several numerical test cases have been performed to prove the efficiency of the approach on different architectures. Sparse direct solvers such as PaStiX are currently limited by their memory requirements and computational cost. They are competitive for small matrices but are often less efficient than iterative methods for large matrices in terms of memory. We are currently accelerating the dense algebra components of direct solvers using hierarchical matrices algebra.

In collaboration with the ICL team from the University of Tennessee, and the STORM team from Inria, we are evaluating the way to replace the embedded scheduling driver of the PaStiX solver by one of the generic frameworks, PaRSEC or StarPU, to execute the task graph corresponding to a sparse factorization. The aim is to design algorithms and parallel programming models for implementing direct methods for the solution of sparse linear systems on emerging computer equipped with GPU accelerators. More generally, this work will be performed in the context of the associate team MORSE and the ANR SOLHAR project which aims at designing high performance sparse direct solvers for modern heterogeneous systems. This ANR project involves several groups working either on the sparse linear solver aspects (HIEPACS and ROMA from Inria and APO from IRIT), on runtime systems (STORM from Inria) or scheduling algorithms (REALOPT and ROMA from Inria). The results of these efforts will be validated in the applications provided by the industrial project members, namely CEA-CESTA and Airbus Group Innovations.

3.3.2. Hybrid direct/iterative solvers based on algebraic domain decomposition techniques

One route to the parallel scalable solution of large sparse linear systems in parallel scientific computing is the use of hybrid methods that hierarchically combine direct and iterative methods. These techniques inherit the advantages of each approach, namely the limited amount of memory and natural parallelization for the iterative component and the numerical robustness of the direct part. The general underlying ideas are not new since they have been intensively used to design domain decomposition techniques; those approaches cover a fairly large range of computing techniques for the numerical solution of partial differential equations (PDEs) in time and space. Generally speaking, it refers to the splitting of the computational domain into sub-domains with or without overlap. The splitting strategy is generally governed by various constraints/objectives but the main one is to express parallelism. The numerical properties of the PDEs to be solved are usually intensively exploited at the continuous or discrete levels to design the numerical algorithms so that the resulting specialized technique will only work for the class of linear systems associated with the targeted PDE.

In that context, we intend to continue our effort on the design of algebraic non-overlapping domain decomposition techniques that rely on the solution of a Schur complement system defined on the interface introduced by the partitioning of the adjacency graph of the sparse matrix associated with the linear system. Although it is better conditioned than the original system the Schur complement needs to be precondition to be amenable to a solution using a Krylov subspace method. Different hierarchical preconditioners will be considered, possibly multilevel, to improve the numerical behaviour of the current approaches implemented in our software libraries HIPS and MaPHyS. This activity will be developed in the context of the ANR DEDALES project. In addition to this numerical studies, advanced parallel implementation will be developed that will involve close collaborations between the hybrid and sparse direct activities.

3.3.3. Linear Krylov solvers

Preconditioning is the main focus of the two activities described above. They aim at speeding up the convergence of a Krylov subspace method that is the complementary component involved in the solvers of interest for us. In that framework, we believe that various aspects deserve to be investigated; we will consider the following ones:

- preconditioned block Krylov solvers for multiple right-hand sides. In many large scientific and industrial applications, one has to solve a sequence of linear systems with several right-hand sides given simultaneously or in sequence (radar cross section calculation in electromagnetism, various source locations in seismic, parametric studies in general, ...). For “simultaneous" right-hand sides, the solvers of choice have been for years based on matrix factorizations as the factorization is performed once and simple and cheap block forward/backward substitutions are then performed. In order to effectively propose alternative to such solvers, we need to have efficient preconditioned Krylov subspace solvers. In that framework, block Krylov approaches, where the Krylov spaces associated with each right-hand side are shared to enlarge the search space will be considered. They are not only attractive because of this numerical feature (larger search space), but also from an implementation point of view. Their block-structures exhibit nice features with respect to data locality and re-usability that comply with the memory constraint of multicore architectures. We will continue the numerical study and design of the block GMRES variant that combines inexact breakdown detection, deflation at restart and subspace recycling. Beyond new numerical investigations, a software implementation to be included in our linear solver libray will be developed in the context of the DGA HIBOX project.
- Extension or modification of Krylov subspace algorithms for multicore architectures: finally to match as much as possible to the computer architecture evolution and get as much as possible performance out of the computer, a particular attention will be paid to adapt, extend or develop numerical schemes that comply with the efficiency constraints associated with the available computers. Nowadays, multicore architectures seem to become widely used, where memory latency and bandwidth are the main bottlenecks; investigations on communication avoiding techniques will be undertaken in the framework of preconditioned Krylov subspace solvers as a general guideline for all the items mentioned above.

3.3.4. Eigensolvers

Many eigensolvers also rely on Krylov subspace techniques. Naturally some links exist between the Krylov subspace linear solvers and the Krylov subspace eigensolvers. We plan to study the computation of eigenvalue problems with respect to the following two different axes:

- Exploiting the link between Krylov subspace methods for linear system solution and eigensolvers, we intend to develop advanced iterative linear methods based on Krylov subspace methods that use some spectral information to build part of a subspace to be recycled, either though space augmentation or through preconditioner update. This spectral information may correspond to a certain part of the spectrum of the original large matrix or to some approximations of the eigenvalues obtained by solving a reduced eigenproblem. This technique will also be investigated in the framework of block Krylov subspace methods.
- In the context of the calculation of the ground state of an atomistic system, eigenvalue computation is a critical step; more accurate and more efficient parallel and scalable eigensolvers are required.

3.4. High performance Fast Multipole Method for N-body problems

Participants: Emmanuel Agullo, Olivier Coulaud, Quentin Khan, Cyrille Piacibello, Guillaume Sylvand.

In most scientific computing applications considered nowadays as computational challenges (like biological and material systems, astrophysics or electromagnetism), the introduction of hierarchical methods based on an octree structure has dramatically reduced the amount of computation needed to simulate those systems for a given accuracy. For instance, in the N-body problem arising from these application fields, we must compute all pairwise interactions among N objects (particles, lines, ...) at every timestep. Among these methods, the Fast Multipole Method (FMM) developed for gravitational potentials in astrophysics and for electrostatic (coulombic) potentials in molecular simulations solves this N-body problem for any given precision with $O(N)$ runtime complexity against $O(N^2)$ for the direct computation.

The potential field is decomposed in a near field part, directly computed, and a far field part approximated thanks to multipole and local expansions. We introduced a matrix formulation of the FMM that exploits the cache hierarchy on a processor through the Basic Linear Algebra Subprograms (BLAS). Moreover, we developed a parallel adaptive version of the FMM algorithm for heterogeneous particle distributions, which is very efficient on parallel clusters of SMP nodes. Finally on such computers, we developed the first hybrid MPI-thread algorithm, which enables to reach better parallel efficiency and better memory scalability. We plan to work on the following points in HIEPACS.

3.4.1. *Improvement of calculation efficiency*

Nowadays, the high performance computing community is examining alternative architectures that address the limitations of modern cache-based designs. GPU (Graphics Processing Units) and the Cell processor have thus already been used in astrophysics and in molecular dynamics. The Fast Mutipole Method has also been implemented on GPU. We intend to examine the potential of using these forthcoming processors as a building block for high-end parallel computing in N-body calculations. More precisely, we want to take advantage of our specific underlying BLAS routines to obtain an efficient and easily portable FMM for these new architectures. Algorithmic issues such as dynamic load balancing among heterogeneous cores will also have to be solved in order to gather all the available computation power. This research action will be conduced on close connection with the activity described in Section 3.2 .

3.4.2. *Non uniform distributions*

In many applications arising from material physics or astrophysics, the distribution of the data is highly non uniform and the data can grow between two time steps. As mentioned previously, we have proposed a hybrid MPI-thread algorithm to exploit the data locality within each node. We plan to further improve the load balancing for highly non uniform particle distributions with small computation grain thanks to dynamic load balancing at the thread level and thanks to a load balancing correction over several simulation time steps at the process level.

3.4.3. *Fast multipole method for dislocation operators*

The engine that we develop will be extended to new potentials arising from material physics such as those used in dislocation simulations. The interaction between dislocations is long ranged ($O(1/r)$) and anisotropic, leading to severe computational challenges for large-scale simulations. Several approaches based on the FMM or based on spatial decomposition in boxes are proposed to speed-up the computation. In dislocation codes, the calculation of the interaction forces between dislocations is still the most CPU time consuming. This computation has to be improved to obtain faster and more accurate simulations. Moreover, in such simulations, the number of dislocations grows while the phenomenon occurs and these dislocations are not uniformly distributed in the domain. This means that strategies to dynamically balance the computational load are crucial to achieve high performance.

3.4.4. *Fast multipole method for boundary element methods*

The boundary element method (BEM) is a well known solution of boundary value problems appearing in various fields of physics. With this approach, we only have to solve an integral equation on the boundary. This implies an interaction that decreases in space, but results in the solution of a dense linear system with $O(N^3)$ complexity. The FMM calculation that performs the matrix-vector product enables the use of Krylov subspace methods. Based on the parallel data distribution of the underlying octree implemented to perform the FMM, parallel preconditioners can be designed that exploit the local interaction matrices computed at the finest level of the octree. This research action will be conduced on close connection with the activity described in Section 3.3 . Following our earlier experience, we plan to first consider approximate inverse preconditionners that can efficiently exploit these data structures.

3.5. Load balancing algorithms for complex simulations

Participants: Astrid Casadei, Olivier Coulaud, Aurélien Esnard, Maria Predari, Pierre Ramet, Jean Roman.

Many important physical phenomena in material physics and climatology are inherently complex applications. They often use multi-physics or multi-scale approaches, which couple different models and codes. The key idea is to reuse available legacy codes through a coupling framework instead of merging them into a stand-alone application. There is typically one model per different scale or physics and each model is implemented by a parallel code.

For instance, to model a crack propagation, one uses a molecular dynamic code to represent the atomistic scale and an elasticity code using a finite element method to represent the continuum scale. Indeed, fully microscopic simulations of most domains of interest are not computationally feasible. Combining such different scales or physics is still a challenge to reach high performance and scalability.

Another prominent example is found in the field of aeronautic propulsion: the conjugate heat transfer simulation in complex geometries (as developed by the CFD team of CERFACS) requires to couple a fluid/convection solver (AVBP) with a solid/conduction solver (AVTP). As the AVBP code is much more CPU consuming than the AVTP code, there is an important computational imbalance between the two solvers.

In this context, one crucial issue is undoubtedly the load balancing of the whole coupled simulation that remains an open question. The goal here is to find the best data distribution for the whole coupled simulation and not only for each stand-alone code, as it is most usually done. Indeed, the naive balancing of each code on its own can lead to an important imbalance and to a communication bottleneck during the coupling phase, which can drastically decrease the overall performance. Therefore, we argue that it is required to model the coupling itself in order to ensure a good scalability, especially when running on massively parallel architectures (tens of thousands of processors/cores). In other words, one must develop new algorithms and software implementation to perform a *coupling-aware* partitioning of the whole application. Another related problem is the problem of resource allocation. This is particularly important for the global coupling efficiency and scalability, because each code involved in the coupling can be more or less computationally intensive, and there is a good trade-off to find between resources assigned to each code to avoid that one of them waits for the other(s). What does furthermore happen if the load of one code dynamically changes relatively to the other one? In such a case, it could be convenient to dynamically adapt the number of resources used during the execution.

There are several open algorithmic problems that we investigate in the HIEPACS project-team. All these problems uses a similar methodology based upon the graph model and are expressed as variants of the classic graph partitioning problem, using additional constraints or different objectives.

3.5.1. *Dynamic load-balancing with variable number of processors*

As a preliminary step related to the dynamic load balancing of coupled codes, we focus on the problem of dynamic load balancing of a single parallel code, with variable number of processors. Indeed, if the workload varies drastically during the simulation, the load must be redistributed regularly among the processors. Dynamic load balancing is a well studied subject but most studies are limited to an initially fixed number of processors. Adjusting the number of processors at runtime allows one to preserve the parallel code efficiency or keep running the simulation when the current memory resources are exceeded. We call this problem, *MxN graph repartitioning*.

We propose some methods based on graph repartitioning in order to re-balance the load while changing the number of processors. These methods are split in two main steps. Firstly, we study the migration phase and we build a “good” migration matrix minimizing several metrics like the migration volume or the number of exchanged messages. Secondly, we use graph partitioning heuristics to compute a new distribution optimizing the migration according to the previous step results.

3.5.2. Load balancing of coupled codes

As stated above, the load balancing of coupled code is a major issue, that determines the performance of the complex simulation, and reaching high performance can be a great challenge. In this context, we develop new graph partitioning techniques, called *co-partitioning*. They address the problem of load balancing for two coupled codes: the key idea is to perform a "coupling-aware" partitioning, instead of partitioning these codes independently, as it is classically done. More precisely, we propose to enrich the classic graph model with *inter-edges*, which represent the coupled code interactions. We describe two new algorithms, and compare them to the naive approach. In the preliminary experiments we perform on synthetically-generated graphs, we notice that our algorithms succeed to balance the computational load in the coupling phase and in some cases they succeed to reduce the coupling communications costs. Surprisingly, we notice that our algorithms do not degrade significantly the global graph edge-cut, despite the additional constraints that they impose.

Besides this, our co-partitioning technique requires to use graph partitioning with *fixed vertices*, that raises serious issues with state-of-the-art software, that are classically based on the well-known recursive bisection paradigm (RB). Indeed, the RB method often fails to produce partitions of good quality. To overcome this issue, we propose a *new* direct k-way greedy graph growing algorithm, called KGGGP, that overcomes this issue and succeeds to produce partition with better quality than RB while respecting the constraint of fixed vertices. Experimental results compare KGGGP against state-of-the-art methods, such as Scotch, for real-life graphs available from the popular *DIMACS'10* collection.

3.5.3. Load balancing strategies for hybrid sparse linear solvers

Graph handling and partitioning play a central role in the activity described here but also in other numerical techniques detailed in sparse linear algebra Section. The Nested Dissection is now a well-known heuristic for sparse matrix ordering to both reduce the fill-in during numerical factorization and to maximize the number of independent computation tasks. By using the block data structure induced by the partition of separators of the original graph, very efficient parallel block solvers have been designed and implemented according to super-nodal or multi-frontal approaches. Considering hybrid methods mixing both direct and iterative solvers such as HIPS or MaPHyS, obtaining a domain decomposition leading to a good balancing of both the size of domain interiors and the size of interfaces is a key point for load balancing and efficiency in a parallel context.

We intend to revisit some well-known graph partitioning techniques in the light of the hybrid solvers and design new algorithms to be tested in the Scotch package.

INDES Project-Team

3. Research Program

3.1. Parallelism, concurrency, and distribution

Concurrency management is at the heart of diffuse programming. Since the execution platforms are highly heterogeneous, many different concurrency principles and models may be involved. Asynchronous concurrency is the basis of shared-memory process handling within multiprocessor or multicore computers, of direct or fifo-based message passing in distributed networks, and of fifo- or interrupt-based event handling in web-based human-machine interaction or sensor handling. Synchronous or quasi-synchronous concurrency is the basis of signal processing, of real-time control, and of safety-critical information acquisition and display. Interfacing existing devices based on these different concurrency principles within HOP or other diffuse programming languages will require better understanding of the underlying concurrency models and of the way they can nicely cooperate, a currently ill-resolved problem.

3.2. Web and functional programming

We are studying new paradigms for programming Web applications that rely on multi-tier functional programming [8]. We have created a Web programming environment named HOP. It relies on a single formalism for programming the server-side and the client-side of the applications as well as for configuring the execution engine.

HOP is a functional language based on the SCHEME programming language. That is, it is a strict functional language, fully polymorphic, supporting side effects, and dynamically type-checked. HOP is implemented as an extension of the BIGLOO compiler that we develop [9]. In the past, we have extensively studied static analyses (type systems and inference, abstract interpretations, as well as classical compiler optimizations) to improve the efficiency of compilation in both space and time.

3.3. Security of diffuse programs

The main goal of our security research is to provide scalable and rigorous language-based techniques that can be integrated into multi-tier compilers to enforce the security of diffuse programs. Research on language-based security has been carried on before in former Inria teams [2], [1]. In particular previous research has focused on controlling information flow to ensure confidentiality.

Typical language-based solutions to these problems are founded on static analysis, logics, provable cryptography, and compilers that generate correct code by construction [6]. Relying on the multi-tier programming language HOP that tames the complexity of writing and analysing secure diffuse applications, we are studying language-based solutions to prominent web security problems such as code injection and cross-site scripting, to name a few.

INFINE Project-Team

3. Research Program

3.1. Online Social Networks (OSN)

Large-scale online social networks such as Twitter or FaceBook provide a powerful means of selecting information. They rely on “social filtering”, whereby pieces of information are collectively evaluated and sorted by users. This gives rise to information cascades when one item reaches a large population after spreading much like an epidemics from user to user in a viral manner. Nevertheless, such OSNs expose their users to a large amount of content of no interest to them, a sign of poor “precision” according to the terminology of information retrieval. At the same time, many more relevant content items never reach those users most interested in them. In other words, OSNs also suffer from poor “recall” performance.

This leads to a first challenge: *what determines the optimal trade-off between precision and recall in OSNs? And what mechanisms should be deployed in order to approach such an optimal trade-off?* We intend to study this question at a theoretical level, by elaborating models and analyses of social filtering, and to validate the resulting hypotheses and designs through experimentation and processing of data traces. More specifically, we envision to reach this general objective by solving the following problems.

3.1.1. Community Detection

Identification of implicit communities of like-minded users and contact recommendation for helping users “rewire” the information network for better performance. Potential schemes may include variants of spectral clustering and belief propagation-style message passing. Limitations / relative merits of candidate schemes, their robustness to noise in the input data, will be investigated.

3.1.2. Incentivization

Design of incentive mechanisms to limit the impact of users’ selfishness on system behavior: efficiency should be maintained even when users are gaming the system to try and increase their estimated expertise. By offering rewards to users on the basis of their involvement in filtering and propagation of content, one might encourage them to adjust their action and contribute to increase the overall efficiency of the OSN as a content access platform.

One promising direction will be to leverage the general class of Vickrey-Clarke-Groves incentive-compatible mechanisms of economic theory to design so-called marginal utility reward mechanisms for OSN users.

3.1.3. Social Recommendation and Privacy

So far we have only alluded to the potential benefits of OSNs in terms of better information access. We now turn to the risks they create. Privacy breaches constitute the greatest of these risks: OSN users disclose a wealth of personal information and thereby expose themselves to discrimination by potential employers, insurers, lenders, government agencies...Such privacy concerns are not specific to OSNs: internauts’ online activity is discretely tracked by companies such as Bluekai, and subsequently monetized to advertisers seeking better ad targeting. While disclosure of personal data creates a privacy risk, on the other hand it fuels personalized services and thereby potentially benefits everyone.

One line of research will be to focus on the specific application scenario of content categorization, and to characterize analytically the trade-off between user privacy protection (captured by differential privacy), accuracy of content categorization, and sample complexity (measured in number of probed users).

3.2. Traffic and Resource Management

Despite the massive increases in transmission capacity of the last few years, one has every reason to believe that networks will remain durably congested, driven among other factors by the steadily increasing demand for video content, the proliferation of smart devices (i.e., smartphones or laptops with mobile data cards), and the forecasted additional traffic due to machine-to-machine (M2M) communications. Despite this rapid traffic growth, there is still a rather limited understanding of the features protocols have to support, the characteristics of the traffic being carried and the context where it is generated. There is thus a strong need for smart protocols that transport requested information at the cheapest possible cost on the network as well as provide good quality of service to network subscribers. One particularly new aspect of up-and-coming networks is that networks are now used to not only (i) access information, but also (ii) distributively process information, en-route.

We intend to study these issues at the theoretical and protocol design levels, by elaborating models and analysis of content demands and/or mobility of network subscribers. The resulting hypothesis and designs will be validated through experimentation, simulation, or data trace processing. It is also worth mentioning the provided solutions may bring benefits to different entities in the network: to content owners (if applied at the core of Internet) or to subscribers or network operators (if applied at the edge of the Internet).

3.2.1. At the Internet Core

One important optimization variable consists in content replication: users can access the closest replica of the content they are interested in. Thus the memory resource can be used to create more replicas and reduce the usage of the bandwidth resource. Another interesting arbitrage between resources arises because content is no longer static but rather dynamic. Here are two simple examples: i) a video could be encoded at several resolutions. There is then a choice between pre-recording all possible resolutions, or alternatively synthesizing a lower-resolution version on the fly from a higher resolution version when a request arises. ii) A user requests the result of a calculation, say the average temperature in a building; this can either be kept in memory, or recomputed each time such a query arises. Optimizing the joint use of all three resources, namely bandwidth, memory, computation, is a complex task. Content Delivery Network companies such as Akamai or Limelight have worked on the memory/bandwidth trade-off for some years, but as we will explain more can be done on this. On the other hand optimizing the memory/computation trade-off has received far less attention. We aim to characterize the best possible content replication strategies by leveraging fine-grained prediction of i) users' future requests, and ii) wireless channels' future bandwidth fluctuations. In the past these two determining inputs have only been considered at a coarse-grained, aggregate level. It is important to assess how much bandwidth saving can be had by conducting finer-grained prediction. We are developing light-weight protocols for conducting these predictions and automatically instantiating the corresponding optimal replication policies. We are also investigating generic protocols for automatically trading replication for computation, focusing initially on the above video transcoding scenario.

3.2.2. At the Internet Edge

Cellular and wireless data networks are increasingly relied upon to provide users with Internet access on devices such as smartphones, laptops or tablets. In particular, the proliferation of handheld devices equipped with multiple advanced capabilities (e.g., significant CPU and memory capacities, cameras, voice to text, text to voice, GPS, sensors, wireless communication) has catalyzed a fundamental change in the way people are connected, communicate, generate and exchange data. In this evolving network environment, users' social relations, opportunistic resource availability, and proximity between users' devices are significantly shaping the use and design of future networking protocols.

One consequence of these changes is that mobile data traffic has recently experienced a staggering growth in volume: Cisco has recently foreseen that the mobile data traffic will increase 18-fold within 2016, in front of a mere 9-fold increase in connection speeds. Hence, one can observe today that the inherently centralized and terminal-centric communication paradigm of currently deployed cellular networks cannot cope with the increased traffic demand generated by smartphone users. This mismatch is likely to last because (1) forecasted mobile data traffic demand outgrows the capabilities of planned cellular technological advances such as 4G or LTE, and (2) there is strong skepticism about possible further improvements brought by 5G technology.

Congestion at the Internet's edge is thus here to stay. Solutions to this problem relates to: densify the infrastructure, opportunistically forward data among neighbors wireless devices, to offload data to alternate networks, or to bring content from the Internet closer to the subscribers. Our recent work on leveraging user mobility patterns, contact and inter-contact patterns, or content demand patterns constitute a starting point to these challenges. The projected increase of mobile data traffic demand pushes towards additional complementary offloading methods. Novel mechanisms are thus needed, which must fit both the new context that Internet users experience now, and their forecasted demands. In this realm, we will focus on new approaches leveraging ultra-distributed, user-centric approaches over IP.

3.3. Spontaneous Wireless Networks (SWN) and Internet of Things (IoT)

The unavailability of end-to-end connectivity in emergent wireless mobile networks is extremely disruptive for IP protocols. In fact, even in simpler cases of spontaneous wireless networks where end-to-end connectivity exists, such networks are still disruptive for the standard IP protocol stack, as many protocols rely on atomic link-local services (such as link-local multicast/broadcast), while these services are inherently unavailable in such networks due to their opportunistic, wireless multi hop nature. In this domain, we will aim to characterize the achievable performance in such IP-disruptive networks and to actively contribute to the design of new, deployable IP protocols that can tolerate these disruptions, while performing well enough compared to what is achievable and remaining interoperable with the rest of the Internet.

Spontaneous wireless networking is also a key aspect of the Internet of Things (IoT). The IoT is indeed expected to massively use this networking paradigm to gradually connect billions of new devices to the Internet, and drastically increase communication without human source or destination – to the point where the amount of such communications will dwarf communications involving humans. Large scale user environment automation require communication protocols optimized to efficiently leverage the heterogeneous and unreliable wireless vicinity (the scope of which may vary according to the application). In fact, extreme constraints in terms of cost, CPU, battery and memory capacities are typically experienced on a substantial fraction of IoT devices. We expect that such constraints will not vanish any time soon for two reasons. On one hand the progress made over the last decade concerning the cost/performance ratio for such small devices is quite disappointing. On the other hand, the ultimate goal of the IoT is ubiquitous Internet connectivity between devices as tiny as dust particles. These constraints actually require to redesign not only the network protocol stack running on these devices, but also the software platform powering these machines. In this context, we will aim at contributing to the design of novel network protocols and software platforms optimized to fit these constraints while remaining compatible with legacy Internet.

3.3.1. Design & Development of Open Experimental IoT Platforms

Manufacturers announce on a regular basis the availability of novel tiny devices, most of them featuring network interfaces: the Internet of Things (IoT) is already here, from the hardware perspective, and it is expected in the near future that we will see a massive increase of the number of muti-purpose smart objects (from tiny sensors in industrial automation to devices like smart watches and tablets). Thus, one of the challenges is to be able to test architectures, protocols and applications, in realistic conditions and at large scale.

One necessity for research in this domain is to establish and improve IoT hardware platforms and testbeds, that integrate representative scenarios (such as Smart Energy, Home Automation etc.) and follow the evolution of technology, including radio technologies, and associated experimentation tools. For that, we plan to build upon the IoT-LAB federated testbeds, that we have participated in designing and deploying recently. We plan to further develop IoT-LAB with more heterogeneous, up-to-date IoT hardware and radios that will provide a usable and realistic experimentation environment. The goal is to provide a tool that enables testing a validation of upcoming software platforms and network stacks targeting concrete IoT deployments.

In parallel, on the software side, IoT hardware available so far made it uneasy for developers to build apps that run across heterogeneous hardware platforms. For instance Linux does not scale down to small, energy-constrained devices, while microcontroller-based OS alternatives were so far rudimentary and yield a steep learning curve and lengthy development life-cycles because they do not support standard programming and debugging tools. As a result, another necessity for research in this domain is to allow the emergence of it more powerful, unifying IOT software platforms, to bridge this gap. For that, we plan to build upon RIOT, a new open source software platform which provides a portable, Linux-like API for heterogeneous IoT hardware. We plan to continue to develop the systems and network stacks aspects of RIOT, within the open source developer community currently emerging around RIOT, which we co-founded together with Freie Universitaet Berlin. The key challenge is to improve usability and add functionalities, while maintaining architectural consistency and a small enough memory footprint. The goal is to provide an IoT software platform that can be used like Linux is used for less constrained machines, both (i) in the context of research and/or teaching, as well as (ii) in industrial contexts. Of course, we plan to use it ourselves for our own experimental research activities in the domain of IoT e.g., as an API to implement novel network protocols running on IoT hardware, to be tested and validated on IoT-LAB testbeds.

3.3.2. Design & Standardization of Architectures and Efficient Protocols for Internet of Things

As described before, and by definition, the Internet of Things will integrate not only a massive number of homogeneous devices (e.g., networks of wireless sensors), but also heterogeneous devices using various communication technologies. Most devices will be very constrained resources (memory resources, computational resources, energy). Communicating with (and amongst) such devices is a key challenge that we will focus on. The ability to communicate efficiently, to communicate reliably, or even just to be able to communicate at all, is non-trivial in many IoT scenarios: in this respect, we intend to develop innovative protocols, while following and contributing to standardization in this area. We will focus and base most of our work on standards developed in the context of the IETF, in working groups such as 6lo, CORE, LWIG etc., as well as IRTF research groups such as NWCRG on network coding and ICNRG on Information Centric Networking. We note however that this task goes far beyond protocol design: recently, radical rearchitecturing of the networks with new paradigms such as Information Centric Networking, ICN, (or even in wired networks, software-defined networks), have opened exciting new avenues. One of our direction of research will be to explore these content-centric approaches, and other novel architectures, in the context of IoT.

KERDATA Project-Team

3. Research Program

3.1. Research axis 1: Convergence of Extreme-Scale Computing and Big Data Infrastructures

The tools and cultures of High Performance Computing and Big Data Analytics have evolved in divergent ways. This is to the detriment of both. However, big computations still generate and are needed to analyze Big Data. As scientific research increasingly depends on both high-speed computing and data analytics, the potential interoperability and scaling convergence of these two eco-systems is crucial to the future. Our objective for the next years is premised on the idea that we must begin to systematically map out and account for the ways in which the major issues associated with Big Data intersect with, impinge upon, and potentially change the plans that are now being laid for achieving Exascale computing.

3.1.1. High-performance storage for concurrent Big Data applications

We argue that storage is a plausible pathway to convergence. In this context, we plan to focus on the needs of concurrent Big Data applications that require high-performance storage, as well as transaction support. Although blobs (binary large objects) are an increasingly popular storage model for such applications, state-of-the-art blob storage systems offer no transaction semantics. This demands users to coordinate data access carefully in order to avoid race conditions, inconsistent writes, overwrites and other problems that cause erratic behavior.

We argue there is a gap between existing storage solutions and application requirements, which limits the design of transaction-oriented applications. In this context, one idea on which we plan to focus our efforts is exploring how blob storage systems could provide built-in, multi-blob transactions, while retaining sequential consistency and high throughput under heavy access concurrency.

The early principles of this research direction have already raised interest from our partners at ANL (Rob Ross) and UPM (María Pérez) for potential collaborations. In this direction, the acceptance of our paper on the Týr transactional blob storage system as a Best Student Paper Award Finalist at the SC16 conference [25] is a very encouraging step.

3.1.2. Big Data analytics on Exascale HPC machines

Big Data analytics is another interesting direction that we plan to explore, building on top of these converged storage architectures. Specifically, we will examine the ways in which Exascale infrastructures can be leveraged not only by HPC-centric, but also by scientific, cloud-centric applications. Many of the current state-of-the-art Big Data processing approaches, including Hadoop and Spark [46] are optimized to run on commodity machines. This impacts the mechanisms used to deal with failures and the limited network bandwidth.

A blind adoption of these systems on extreme-scale platforms would result in high overheads. It would therefore prevent users from fully benefiting from the high performance infrastructure. The objective that we set here is to explore design and implementation options for new data analytics systems that can exploit the features of extreme-scale HPC machines: multi-core nodes, multiple memory and storage technologies including a large memory, NVRAM, SSDs, etc.

Collaboration. *This axis is addressed in close collaboration with María Pérez (UPM), Rob Ross (ANL), Toni Cortes (BSC), Bogdan Nicolae (formerly at IBM Research, now at Huawei Research).*

Relevant groups with similar interests are the following ones.

- *The group of Jack Dongarra, Innovative Computing Laboratory at University of Tennessee/Oak Ridge National Laboratory, working on joint tools Exascale Computing and Big Data.*
- *The group of Satoshi Matsuoka, Tokyo Institute of Technology, working on system software for Clouds and HPC.*
- *The group of Franck Cappello at Argonne National Laboratory/NCSA working on on-demand data analytics and storage for extreme-scale simulations and experiments.*

3.2. Research axis 2: Advanced data processing on Clouds

The recent evolutions in the area of Big Data processing have pointed out some limitations of the initial Map-Reduce model. It is well suited for batch data processing, but less suited for real-time processing of dynamic data streams. New types of data-intensive applications emerge, e.g., for enterprises who need to perform analysis on their stream data in ways that can give fast results (i.e., in real time) at scale (e.g., click-stream analysis and network-monitoring log analysis). Similarly, scientists require fast and accurate data processing techniques in order to analyze their experimental data correctly at scale (e.g., collectively analysis of large data sets distributed in multiple geographically distributed locations).

Our plan is to revisit current data management techniques to cope with the volatile requirements of data-intensive applications on large-scale dynamic clouds in a cost-efficient way.

3.2.1. Stream-oriented, Big Data processing on clouds

The state-of-the-art Hadoop Map-Reduce framework cannot deal with stream data applications, as it requires the data to be initially stored in a distributed file system in order to process them. To better cope with the above-mentioned requirements, several systems have been introduced for stream data processing such as Flink [41], Spark [46], Storm [47], and Google MillWheel [49]. These systems keep computation in memory to decrease latency, and preserve scalability by using data-partitioning or dividing the streams into a set of deterministic batch computations.

However, they are designed to work in dedicated environments and they do not consider the performance variability (i.e., network, I/O, etc.) caused by resource contention in the cloud. This variability may in turn cause high and unpredictable latency when output streams are transmitted to further analysis. Moreover, they overlook the dynamic nature of data streams and the volatility in their computation requirements. Finally, they still address failures in a best-effort manner.

Our objective is to investigate new approaches for reliable, stream Big Data processing on clouds. We will explore new mechanisms that expose resource heterogeneity (observed variability in resource utilization at runtime) when scheduling stream data applications. We will also investigate how to adapt to node failures automatically, and to adapt the failure handling techniques to the characteristics of the running application and to the root cause of failures.

3.2.2. Geographically distributed workflows on multi-site clouds

Many data processing jobs in data-intensive applications are modeled as workflows (i.e., as sets of tasks linked according to their data and computation dependencies) to facilitate the management and analysis of large volumes of data. With the fast growth of volumes of data to be handled at larger and larger scales, geographically distributed workflows are emerging as a natural data processing paradigm. This may bring several benefits: resilience to failures, distribution across partitions (e.g., moving computation close to data or vice versa), elastic scaling to support usage bursts, user proximity, etc.

In this context, sharing, disseminating and analyzing the data sets results in frequent large-scale data movements across widely distributed sites. Studies show that the inter-datacenter traffic is expected to triple in the following years. Our objective is to investigate approaches to data management enabling an efficient execution of such geographically distributed workflows running on multi-site clouds.

While in the past years we have addressed some data management issues in this area, mainly in support to efficient task scheduling of scientific workflows running on multisite clouds, we will now focus on an increasingly common scenario where workflows generate and process a huge number of small files, which is particularly challenging. As such workloads generate a deluge of small and independent I/O operations, efficient data and metadata handling is critical. We will explore specific means to better hide latency for data and metadata access in such scenarios, as a way to improve global performance.

Collaboration. *This axis is addressed in close collaboration with María Pérez (UPM), Kate Keahey (ANL) and Toni Cortes (BSC).*

Relevant groups with similar interests include the following ones.

- *The AMPLab, UC Berkeley, USA, working on scheduling stream data applications in heterogeneous clouds.*
- *The group of Ewa Deelman, USC Information Sciences Institute, working on resource management for workflows in Clouds.*
- *The XTRA group, Nanyang Technological University, Singapore, working on resource provisioning for workflows in the cloud.*

3.3. Research axis 3: I/O management, in situ visualization and analysis on HPC systems at extreme scales

Over the past few years, the increasing amounts of data produced by large-scale simulations have motivated a shift from traditional offline data analysis to in situ analysis and visualization. In situ processing started by coupling a parallel simulation with an analysis or visualization library, to avoid the cost of writing data on storage and reading it back. Going beyond this simple pairwise tight coupling, complex analysis workflows today are graphs with one or more data sources and several interconnected analysis components.

3.3.1. Toward a joint optimized architecture for in situ visualization and advanced processing

From Inria and ANL, four tools at least have emerged to address some challenges of coupling simulations with visualization packages or analysis workflows. Each of them focused on some particular aspect:

Damaris (Inria, [12], [4]) exploits dedicated cores to enable jitter-free I/O and in situ visualization;

Decaf (ANL, [36]) implements a coupling service for workflows;

FlowVR (Inria, [48]) connects workflow components for in situ processing;

Swift (ANL, [51]) focuses on implicitly parallel data flows and was optimized for Big Data processing.

Our plan is to explore how these tools could best leverage their respective strengths in a *joint optimized architecture for in situ visualization and advanced processing* in the HPC area. We published a preliminary study describing the lessons learned from using these tools in production environments with real applications [6]. Such a joint architecture will contribute to address the data volume and velocity challenges raised by data-intensive workflows, including complex data-intensive analytics phases. It may also impact, in a subsequent step, future data analysis pipelines for converged Big Data and HPC architectures.

Collaboration. *This axis is worked out in close collaboration with Rob Ross (ANL), Tom Peterka (ANL), Matthieu Dorier (ANL), Toni Cortes (BSC), Bruno Raffin (Inria). Some additional collaborations are in discussion with other members of JLESC, and with CEA and Total.*

Relevant groups with similar interests include the following ones.

- *The group of Manish Parashar at Rutgers University, USA (I/O management for HPC systems, in situ processing).*
- *The group of Scott Klasky at Oak Ridge National Lab, USA (I/O management for HPC systems, in situ processing).*
- *The CNRS IPSL laboratory (Sébastien Denvil, Pôle de modélisation du climat) in Paris, France (in situ data analytics).*

MADYNES Project-Team

3. Research Program

3.1. Evolutionary needs in network and service management

The foundation of the MADYNES research activity is the ever increasing need for automated monitoring and control within networked environments. This need is mainly due to the increasing dependency of both people and goods towards communication infrastructures as well as the growing demand towards services of higher quality. Because of its strategic importance and crucial requirements for interoperability, the management models were constructed in the context of strong standardization activities by many different organizations over the last 15 years. This has led to the design of most of the paradigms used in today's deployed approaches. These paradigms are the Manager/Agent interaction model, the Information Model paradigm and its container, together with a naming infrastructure called the Management Information Base. In addition to this structure, five functional areas known under Fault, Configuration, Accounting, Performance and Security are associated to these standards.

While these models were well suited for the specific application domains for which they were designed (telecommunication networks or dedicated protocol stacks), they all show the same limits. Especially they are unable:

1. to deal with any form of dynamicity in the managed environment,
2. to master the complexity, the operating mode and the heterogeneity of the emerging services,
3. to scale to new networks and service environments.

These three limits are observed in all five functional areas of the management domain (fault, configuration, accounting, performance and security) and represent the major challenges when it comes to enable effective automated management and control of devices, networks and services in the next decade.

MADYNES addresses these challenges by focusing on the design of management models that rely on inherently dynamic and evolving environments. The project is centered around two core activities. These activities are, as mentioned in the previous section, the design of an autonomous management framework and its application to three of the standard functional areas namely security, configuration and performance.

MAESTRO Project-Team

3. Research Program

3.1. Research Directions

MAESTRO's research directions belong to five main themes motivated by direct applications: network science, wireless networks, network engineering games, green networking and smart grids, content-oriented systems. These directions are very connected: network engineering games find applications in many networking fields, from wireless protocols to applications such as social networks. Green IT studies are often concerned with wireless networks, etc. The study of these applications often raises questions of methodological nature, less close to direct applications; these advances are reported in a separate section.

3.1.1. Network Science

MAESTRO contributes to this new fast growing research subject. "Network Science" or "Complex Network Analysis" aims at understanding the structural properties and the dynamics of a variety of large-scale networks in telecommunications (e.g. the graph of autonomous systems, the Web graph), social science (e.g. community of interest, advertisement, reputation, recommendation systems), bibliometrics (e.g. citations, co-authors), biology (e.g. spread of an epidemic, protein-protein interactions), and physics. It has been observed that the complex networks encountered in these areas share common properties such as power law degree distribution, small average distances, community structure, etc. It also appears that many general questions/applications (e.g. community detection, epidemic spreading, search, anomaly detection) are common in various disciplines which study networks. In particular, we aim at understanding the evolution of complex networks with the help of game theoretical tools in connection with Network Engineering Games, as described below. We design efficient tools for measuring specific properties of large scale complex networks and their dynamics. More specifically, we work on the problem of distributed optimization in large networks where nodes cooperatively solve an optimization problem relying only on local information exchange.

3.1.2. Wireless Networks

The amazing technological advances in wireless devices has led networks to become heterogeneous and very complex. Many research groups worldwide investigate performance evaluation of wireless technologies. MAESTRO's specificity relies on the use of a large variety of analytic tools from applied probability, control theory and distributed optimization to study and improve wireless networks functionalities. We investigate in particular problems of self-organization, channel selection and power control, the association problem and others.

3.1.3. Network Engineering Games

The foundations of *Network Engineering Games* are currently being laid. These are games arising in telecommunications engineering at all the networking layers. This includes considerations from information and communications theory for dealing with the physical and link layers, along with cross layer approaches. MAESTRO's focus is on three areas: *routing games*, *evolutionary games* and *epidemic games*. In routing games we progress on the theory for costs that are not additive over links (such as packet losses or call blocking probabilities). We pursue their research in the stochastic extension of evolutionary game theory, namely the "anonymous sequential games" in which we study the total expected costs and the average cost. Within epidemic games they study epidemics that compete against each other. We apply this to social networks, considering in particular the coupling between various social networks (e.g. propagation strategies that combine Twitter, FaceBook and other social networks).

3.1.4. Green Networking and Smart Grids

The ICT (Information and Communications Technology) sector is becoming one of the main energy consumers worldwide. There is awareness that networks should have a reduced environmental footprint. Our objective is to have a systematically "green" approach when solving optimization problems. The energy cost and the environmental impact should be considered in optimization functions along with traditional performance metrics such as throughput, fairness or delay. We aim at contributing to the design and the analysis of future green networks, in particular those using renewable energy.

Researchers envision that future electricity distribution network will be "smart", with a large number of small generators (due to an extensive use of renewable energies) and of consumer devices able to adapt their energy needs to a time-varying offer. Generators and devices will be able to locally communicate through the electrical grid itself (or more traditional communication networks), in order to optimize production, transport and use of the energy. This is definitely a new application scenario for MAESTRO, to which we hope to be able to contribute with our expertise on analytic models and performance evaluation.

3.1.5. Content-Oriented Systems

We generally study problems related with the placement and the retrieval of data in communication networks.

We are particularly interested in In-network caching, a widely adopted technique to provide an efficient access to data or resources on a world-wide deployed system while ensuring scalability and availability. For instance, caches are integral components of the Domain Name System, the World Wide Web, Content Distribution Networks, or the recently proposed Information-Centric Network (ICN) architectures. We analyze network of caches, study their optimal placement in the network and optimize data placement in caches/servers.

We also study other aspects related to replication and placement of data: how much to replicate it and on which servers to place it? Finally, we study optimal ways of retrieving the data through prefetching.

3.1.6. Advances in Methodological Tools

MAESTRO has a methodological activity that aims at advancing the state of the art in the tools used for the general performance evaluation and control of systems. We contribute to such fields as perturbation analysis, Markov processes, queueing theory, control theory and game theory. Another objective is to enhance our activity on general-purpose modeling algorithms and software for controlled and uncontrolled stochastic systems.

3.2. Scientific Foundations

The main mathematical tools and formalisms used in MAESTRO include:

- theory of stochastic processes: Markov process, renewal process, branching process, point process, Palm measure, large deviations, mean-field approximation, fluid approximation;
- theory of dynamical discrete-event systems: queues, pathwise and stochastic comparisons, random matrix theory;
- theory of control and scheduling: dynamic programming, Markov decision process, game theory, deterministic and stochastic scheduling; stochastic approximation algorithms;
- theory of singular perturbations.

MIMOVE Team

3. Research Program

3.1. Introduction

MiMove targets research enabling next-generation mobile distributed systems, from their conception and design to their runtime support. These systems are challenged by their own success and consequent massive growth, as well as by the present and future, fast evolving, global networking and computing environment. This context is well-captured by the Future Internet vision, whose mobile constituents are becoming the norm rather than the exception. MiMove's research topics relate to a number of scientific domains with intensive ongoing research, such as ubiquitous computing, self-adaptive systems, wireless sensor networks, participatory sensing and social networks. In the following, we discuss related state-of-the-art research – in particular work focusing on middleware for mobile systems – and we identify the open research challenges that drive our work.

3.2. Emergent mobile distributed systems

Emergent mobile distributed systems promise to provide solutions to the complexity of the current and future computing and networking environments as well as to the ever higher demand for ubiquitous mobile applications, in particular being a response to the volatile and evolving nature of both the former and the latter. Hence, such systems have gained growing interest in the research literature. Notably, research communities have been formed around *self-adaptive systems* and *autonomic systems*, for which various overlapping definitions exist [72]. Self-adaptive systems are systems that are able to adapt themselves to uncertain execution environments, while autonomic systems have been defined as having one or more characteristics known as *self-** properties, including self-configuring, self-healing, self-optimizing and self-protecting [54]. Self-adaptive or autonomic systems typically include an adaptation loop comprising *modeling*, *monitoring*, *analyzing*, *deciding* and *enactment* processes. The adaptation loop provides feedback about changes in the system and its environment to the system itself, which adjusts itself in response. Current research on emergent distributed systems, including mobile ones, addresses all the dimensions of the adaptation loop [31], [25], [61], [83].

In our previous work, we introduced the paradigm of *emergent middleware*, which enables networked systems with heterogeneous behaviors to coordinate through adequate interaction protocols that emerge in an automated way [50], [28], [26]. A key point of that work is the combined study of the application- and middleware-layer behaviors, while current efforts in the literature tend to look only at one layer, either the application [48] or the middleware [19], [49], and take the other for granted (i.e., homogeneous, allowing direct coordination). Furthermore, the uncertainty of the computing and networking environments that is intrinsic to emergent mobile distributed systems [41] calls for taking into account also the underlying network and computational resources in a cross-layer fashion. In another line of work, we studied cross-integration of heterogeneous interaction paradigms at the middleware layer (message passing versus event-based and data sharing), where we investigate functional and QoS semantics of paradigms across their interconnections [43], [53]. Our focus there is to grasp the relation between individual and end-to-end semantics when bridging heterogeneous interaction protocols. In contrast, existing research efforts typically focus on emergent or evolving properties in homogeneous settings [42]. Last but not least, integrating heterogeneous mobile distributed systems into emergent compositions raises the question of dependability. More specifically, the overall correctness of the composition with respect to the individual requirements of the constituent systems can be particularly hard to ensure due to their heterogeneity. Again, current approaches typically deal with homogeneous constraints for dependability [39], [85], [40] with few exceptions [38].

As evident from the above, there is considerable interest and intensive research on emergent mobile distributed systems, while at the same time there are key research questions that remain open despite initial relevant work, including ours, which are summarized in the following:

- How to effectively deal with the combined impact on emergent properties of the different functional layers of mobile distributed systems (e.g., [50], [28], [26], [69])?
- How to perceive and model emergent properties in space and in time across volatile compositions of heterogeneous mobile distributed systems (e.g., [43], [53])?
- How to produce dependable emergent mobile distributed systems, i.e., systems that correctly meet their requirements, despite uncertainty in their emergence and execution exacerbated by heterogeneity (e.g., [38])?

3.3. Large-scale mobile sensing and actuation

In the past decade, the increasingly low cost of MEMS [0] devices and low-power microprocessors has led to a significant amount of research into mobile sensing and actuation. The results of this are now reaching the general public, going beyond the largely static use of sensors in scenarios such as agriculture and waste-water management, into increasingly *mobile* systems. These include sensor-equipped smartphones and personal wearable devices focused on the idea of a “quantified self", gathering data about a user’s daily habits in order to enable them to improve their well-being. However, in spite of significant advances, the key challenges of these systems arise from largely the same attributes as those of early envisioned mobile systems, introduced in [76] and re-iterated in [75]: relative resource-poverty in terms of computation and communication, variable and unreliable connectivity, and limitations imposed by a finite energy source. These remain true even though modern mobile devices are significantly more powerful compared to their ancestors; the work we expect them to do has increased, and the computation and storage abilities available through fixed infrastructure such as the cloud are larger by order of magnitudes than any single mobile device. The design of algorithms and protocols to efficiently coordinate the sensing, processing, and actuation capabilities of the large number of mobile devices in future systems is a core area of MiMove’s research.

Precisely, the focus of MiMove’s research interests lies mostly in the systems resulting from the increased popularity of sensor-equipped smart devices that are carried by people, which has led to the promising field of *mobile phone sensing* or *mobile crowd-sensing* [58], [55]. The paradigm is powerful, as it allows overcoming the inherent limitation of traditional sensing techniques that require the deployment of dedicated fixed sensors (e.g., see work on noise mapping using the microphones in users’ telephones [70]). Specifically, we are interested in the challenges below, noting that initial work to address them already exists, including that by team members:

- How to efficiently manage the large scale that will come to the fore when millions, even billions of devices will need to be managed and queried simultaneously (e.g., [81], [45])?
- How to efficiently coordinate the available devices, including resource-poor mobile devices and the more-capable cloud infrastructure (e.g., [68], [36], [74], [64])?
- How to guarantee dependability in a mobile computing environment (e.g., [34], [80], [30])?
- How to ensure that the overhead of sensing does not lead to a degraded performance for the user (e.g., [56], [36])?

3.4. Mobile social crowd-sensing

Mobile crowd-sensing as introduced in Section 3.3 is further undergoing a transformation due to the widespread adoption of social networking. The resulting mobile *social* crowd-sensing may be qualified as “*people-centric sensing*” and roughly subdivides into two categories [57]: i) *participatory sensing*, and ii) *opportunistic sensing*. Participatory sensing entails direct involvement of humans controlling the mobile devices, while opportunistic sensing requires the mobile device itself to determine whether or not to perform

[0] Micro-Electro-Mechanical Systems.

the sensing task. Orthogonally to the above categorization, mobile sensing can be [55]: i) *personal sensing*, mostly to monitor a person's context and well-being; ii) *social sensing*, where updates are about the social and emotional statuses of individuals; or iii) *urban (public) sensing*, where public data is generated by the public and for the public to exploit. Personal sensing is aimed towards personal monitoring and involves one or just a few devices in direct relationship with their custodian. For instance, SoundSense [62] is a system that enables each person's mobile device to learn the types of sounds the owner encounters through unsupervised learning. Another application example relates to the sensing-based detection of the users' transportation mode by using their smartphones [47]. In social sensing, the mobile device or its owner decides what social information to share about the owner or the owner's environment, with an individual or group of friends [55], [37], [52], [21], [66]. Social sensing is mostly participatory. Therefore, it is the custodian of the device who determines when and where data should be generated. Social participatory sensing is closely related to social networking [63]. On the other hand, within opportunistic social sensing, the underlying system is in charge of acquiring needed data through relevant probes, as opposed to having the end-user providing them explicitly [24], [51], [22]. In urban sensing, also known as public sensing, data can be generated by everyone (or their devices) and exploited by everyone for public knowledge, including environment monitoring, or traffic updates [55]. In participatory urban sensing, users participate in providing information about the environment by exploiting the sensors/actuators embedded in their devices (which can be smartphones, vehicles, tablets, etc.) [55]. However data is only generated according to the owner's willingness to participate. Participatory urban sensing is especially characterized by scale issues at the data level, where data is generated by numerous individuals and should be processed and aggregated for knowledge to be inferred, involving adequate data scaling approaches [44]. Ikarus [84] is an example of participatory sensing, where data is collected by a large number of paragliders throughout their flights. The focus is on aggregating the data and rendering the results on a thermal map.

As outlined above, mobile social crowd-sensing has been a very active field of research for the last few years with various applications being targeted. However, effectively enabling mobile social crowd-sensing still raises a number of challenges, for which some early work may be identified:

- How to ensure that the system delivers the right quality of service, e.g., in terms of user-perceived delay, in spite of the resource constraints of mobile systems (e.g., [71])?
- How to guarantee the right level of privacy (e.g., [33], [73])?
- How to ensure the right level of participation from end-users so that mobile sensing indeed becomes a relevant source of accurate knowledge, which relates to eliciting adequate incentive mechanisms [86], in particular based on the understanding of mobile application usage [78], [77]?
- How to enrich sensor-generated content that is quantitative with user-generated one, thereby raising the issue of leveraging highly unstructured data while benefiting from a rich source of knowledge (e.g., sensing the crowdedness of a place combined with the feeling of people about the crowdedness, which may hint on the place's popularity as much as on discomfort)?

MUSE Team

3. Research Program

3.1. Active probing methods

We are developing methods that actively introduce probes in the network to discover properties of the connected devices and network segments. We are focusing in particular on methods to discover properties of home networks (connected devices and their types) and to distinguish if performance bottlenecks lie within the home network versus outside. Our goal is to develop adaptative methods that can leverage the collaboration of the set of available devices (including end-user devices and the home router, depending on which devices are running the measurement software).

3.2. Passive monitoring methods

This part our research develops methods that simply observe network traffic to infer the performance of networked applications and the location of performance bottlenecks, as well as to extract patterns of web content consumption. We are working on techniques to collect network traffic both at user's end-devices and at home routers. We also have access to network traffic traces collected on a campus network and on a large European broadband access provider.

3.3. Inferring user online experience

We are developing hybrid measurement methods that combine passive network measurement techniques to infer application performance with techniques from HCI to measure user perception. We will later use the resulting datasets to build models of user perception of network performance based only on data that we can obtain automatically from the user device or from user's traffic observed in the network.

3.4. Filtering real-time Web streams

The Web has become a large-scale real-time information system forcing us to revise both how to effectively assess relevance of information for a user and how to efficiently implement information retrieval and dissemination functionality. To increase information relevance, Real-time Web applications such as Twitter and Facebook, extend content and social-graph relevance scores with "real-time" user generated events (e.g. re-tweets, replies, likes). To accommodate high arrival rates of information items and user events we explore a publish/subscribe paradigm in which we index queries and update on the fly their results each time a new item and relevant events arrive. In this setting, we need to process continuous top-k text queries combining both static and dynamic scores. To the best of our knowledge, this is the first work addressing how non-predictable, dynamic scores can be handled in a continuous top-k query setting.

3.5. Flexible online drift detection

Monitoring streaming content is a challenging big data analytics problem, given that very large datasets are rarely (if ever) stationary. In several real world monitoring applications (e.g., newsgroup discussions, network connections, etc.) we need to detect significant change points in the underlying data distribution (e.g., frequency of words, sessions, etc.) and track the evolution of those changes over time. These change points, depending on the research community, are referred to as temporal evolution, non-stationarity, or concept drift and provide valuable insights on real world events (e.g. a discussion topic, an intrusion) to take a timely action. In our work, we adopt a query-based approach to drift detection and address the question of processing drift queries over very large datasets. To the best of our knowledge, our work is the first to formalize flexible drift queries on streaming datasets with varying change rates.

MYRIADS Project-Team

3. Research Program

3.1. Introduction

In this section, we present our research challenges along four work directions: resource and application management in distributed cloud architectures for scaling clouds in Section 3.2 , energy management strategies for greening clouds in Section 3.3 , security and data protection aspects for securing cloud-based information systems and applications in Section 3.4 , and methods for experimenting with clouds in Section 3.5 .

3.2. Scaling clouds

3.2.1. Resource management in hierarchical clouds

The next generation of utility computing appears to be an evolution from highly centralized clouds towards more decentralized platforms. Today, cloud computing platforms mostly rely on large data centers servicing a multitude of clients from the edge of the Internet. Servicing cloud clients in this manner suggests that locality patterns are ignored: wherever the client issues his/her request from, the request will have to go through the backbone of the Internet provider to the other side of the network where the data center relies. Besides this extra network traffic and this latency overhead that could be avoided, other common centralization drawbacks in this context stand in limitations in terms of security/legal issues and resilience.

At the same time, it appears that network backbones are over-provisioned for most of their usage. This advocates for placing computing resources directly within the backbone network. The general challenge of resource management for such clouds stands in trying to be locality-aware: for the needs of an application, several virtual machines may exchange data. Placing them *close* to each others can significantly improve the performance of the application they compose. More generally, building an overlay network which takes the hierarchical aspects of the platform without being a hierarchical overlay – which comes with load balancing and resilience issues is a challenge by itself.

The results of these works are planned to be integrated into the Discovery initiative [52] which aims at revisiting OpenStack to offer a cloud stack able to manage utility computing platforms where computing resources are located in small computing centers in the backbone's PoPs (Point of Presence) and interconnected through the backbone's internal links.

3.2.2. Resource management in mobile edge clouds

Mobile edge cloud (MEC) infrastructures are composed of compute, storage and networking resources located at the edge of wide-area networks, in immediate proximity to the end users. Instead of treating the mobile operator's network as a high-latency dumb pipe between the end users and the external service providers, MEC platforms aim at deploying cloud functionalities *within* the mobile phone network, inside or close to the mobile access points. Doing so is expected to deliver added value to the content providers and the end users by enabling new types of applications ranging from Internet-of-Things applications to extremely interactive systems (e.g., augmented reality). Simultaneously, it will generate extra revenue streams for the mobile network operators, by allowing them to position themselves as cloud computing operators and to rent their already-deployed infrastructure to content and application providers.

Mobile edge clouds have very different geographical distribution compared to traditional clouds. While traditional clouds are composed of many reliable and powerful machines located in a very small number of data centers and interconnected by very high-speed networks, mobile edge cloud are composed of a very large number of points-of-presence with a couple of weak and potentially unreliable servers, interconnected with each other by commodity long-distance networks. This creates new demands for the organization of a scalable mobile edge computing infrastructure, and opens new directions for research.

The main challenges that we plan to address are:

- How should an edge cloud infrastructure be designed such that it remains scalable, fault-tolerant, controllable, energy-efficient, etc.?
- How should applications making use of edge clouds be organized? One promising direction is to explore the extent to which stream-data processing platforms such as Apache Spark and Apache Flink can be adapted to become one of the main application programming paradigms in such environments.

3.2.3. Self-optimizing applications in multi-cloud environments

As the use of cloud computing becomes pervasive, the ability to deploy an application on a multi-cloud infrastructure becomes increasingly important. Potential benefits include avoiding dependence on a single vendor, taking advantage of lower resource prices or resource proximity, and enhancing application availability. Supporting multi-cloud application management involves two tasks. First, it involves selecting an initial multi-cloud application deployment that best satisfies application objectives and optimizes performance and cost. Second, it involves dynamically adapting the application deployment in order to react to changes in execution conditions, application objectives, cloud provider offerings, or resource prices. Handling price changes in particular is becoming increasingly complex. The reason is the growing trend of providers offering sophisticated, dynamic pricing models that allow buying and selling resources of finer granularities for shorter time durations with varying prices.

Although multi-cloud platforms are starting to emerge, these platforms impose a considerable amount of effort on developers and operations engineers, provide no support for dynamic pricing, and lack the responsiveness and scalability necessary for handling highly-distributed, dynamic applications with strict quality requirements. The goal of this work is to develop techniques and mechanisms for automating application management, enabling applications to cope with and take advantage of the dynamic, diverse, multi-cloud environment in which they operate.

The main challenges arising in this context are:

- selecting effective decision-making approaches for application adaptation,
- supporting scalable monitoring and adaptation across multiple clouds,
- performing adaptation actions in a cost-efficient and safe manner.

3.3. Greening clouds

ICT (Information and Communications Technologies) ecosystem now approaches 5% of world electricity consumption and this ICT energy use will continue grow fast because of the information appetite of Big Data, big networks and big infrastructures as Clouds that unavoidably leads to big power.

3.3.1. Smart grids and clouds

We propose exploiting Smart Grid technologies to come to the rescue of energy-hungry Clouds. Unlike in traditional electrical distribution networks, where power can only be moved and scheduled in very limited ways, Smart Grids dynamically and effectively adapt supply to demand and limit electricity losses (currently 10% of produced energy is lost during transmission and distribution).

For instance, when a user submits a Cloud request (such as a Google search for instance), it is routed to a data center that processes it, computes the answer and sends it back to the user. Google owns several data centers spread across the world and for performance reasons, the center answering the user's request is more likely to be the one closest to the user. However, this data center may be less energy efficient. This request may have consumed less energy, or a different kind of energy (renewable or not), if it had been sent to this further data center. In this case, the response time would have been increased but maybe not noticeably: a different trade-off between quality of service (QoS) and energy-efficiency could have been adopted.

While Clouds come naturally to the rescue of Smart Grids for dealing with this big data issue, little attention has been paid to the benefits that Smart Grids could bring to distributed Clouds. To our knowledge, no previous work has exploited the Smart Grids potential to obtain and control the energy consumption of entire Cloud infrastructures from underlying facilities such as air conditioning equipment (which accounts for 30% to 50% of a data center's electricity bill) to network resources (which are often operated by several actors) and to computing resources (with their heterogeneity and distribution across multiple data centers). We aim at taking advantage of the opportunity brought by the Smart Grids to exploit renewable energy availability and to optimize energy management in distributed Clouds.

3.3.2. Energy cost models

Cloud computing allows users to outsource the computer resources required for their applications instead of using a local installation. It offers on-demand access to the resources through the Internet with a pay-as-you-go pricing model.However, this model hides the electricity cost of running these infrastructures.

The costs of current data centers are mostly driven by their energy consumption (specifically by the air conditioning, computing and networking infrastructure). Yet, current pricing models are usually static and rarely consider the facilities' energy consumption per user. The challenge is to provide a fair and predictable model to attribute the overall energy costs per virtual machine and to increase energy-awareness of users.

Another goal consists in better understanding the energy consumption of computing and networking resources of Clouds in order to provide energy cost models for the entire infrastructure including incentivizing cost models for both Cloud providers and energy suppliers. These models will be based on experimental measurement campaigns on heterogeneous devices. Inferring a cost model from energy measurements is an arduous task since simple models are not convincing, as shown in our previous work. We aim at proposing and validating energy cost models for the heterogeneous Cloud infrastructures in one hand, and the energy distribution grid on the other hand. These models will be integrated into simulation frameworks in order to validate our energy-efficient algorithms at larger scale.

3.3.3. Energy-aware users

In a Cloud moderately loaded, some servers may be turned off when not used for energy saving purpose. Cloud providers can apply resource management strategies to favor idle servers. Some of the existing solutions propose mechanisms to optimize VM scheduling in the Cloud. A common solution is to consolidate the mapping of the VMs in the Cloud by grouping them in a fewer number of servers. The unused servers can then be turned off in order to lower the global electricity consumption.

Indeed, current work focuses on possible levers at the virtual machine suppliers and/or services. However, users are not involved in the choice of using these levers while significant energy savings could be achieved with their help. For example, they might agree to delay slightly the calculation of the response to their applications on the Cloud or accept that it is supported by a remote data center, to save energy or wait for the availability of renewable energy. The VMs are black boxes from the Cloud provider point of view. So, the user is the only one to know the applications running on her VMs.

We plan to explore possible collaborations between virtual machine suppliers, service providers and users of Clouds in order to provide users with ways of participating in the reduction of the Clouds energy consumption. This work will follow two directions: 1) to investigate compromises between power and performance/service quality that cloud providers can offer to their users and to propose them a variety of options adapted to their workload; and 2) to develop mechanisms for each layer of the Cloud software stack to provide users with a quantification of the energy consumed by each of their options as an incentive to become greener.

3.4. Securing clouds

3.4.1. Security monitoring SLO

While the trend for companies to outsource their information system in clouds is confirmed, the problem of securing an information system becomes more difficult. Indeed, in the case of infrastructure clouds, physical resources are shared between companies (also called tenants) but each tenant controls only parts of the shared resources, and, thanks to virtualization, the information system can be dynamically and automatically reconfigured with added or removed resources (for example starting or stopping virtual machines), or even moved between physical resources (for example using virtual machine migration). Partial control of shared resources brings new classes of attacks between tenants, and security monitoring mechanisms to detect such attacks are better placed out of the tenant-controlled virtual information systems, that is under control of the cloud provider. Dynamic and automatic reconfigurations of the information system make it unfeasible for a tenant's security administrator to setup the security monitoring components to detect attacks, and thus an automated self-adaptable security monitoring service is required.

Combining the two previous statements, there is a need for a dependable, automatic security monitoring service provided to tenants by the cloud provider. Our goal is to address the following challenges to design such a security monitoring service:

1. to define relevant Service-Level Objectives (SLOs) of a security monitoring service, that can figure in the Service-Level Agreement (SLA) signed between a cloud provider and a tenant;
2. to design heuristics to automatically configure provider-controlled security monitoring software components and devices so that SLOs are reached, even during automatic reconfigurations of tenants' information systems;
3. to design evaluation methods for tenants to check that SLOs are reached.

Moreover in challenges 2 and 3 the following sub-challenges must be addressed:

- although SLAs are bi-lateral contracts between the provider and each tenant, the implementation of the contracts is based on shared resources, and thus we must study methods to combine the SLOs;
- the designed methods should have a minimal impact on performance.

3.4.2. Data Protection in Cloud-based IoT Services

The Internet of Things is becoming a reality. Individuals have their own swarm of connected devices (e.g. smartphone, wearables, and home connected objects) continually collecting personal data. A novel generation of services is emerging exploiting data streams produced by the devices' sensors. People are deprived of control of their personal data as they don't know precisely what data are collected by service providers operating on Internet (oISP), for which purpose they could be used, for how long they are stored, and to whom they are disclosed. In response to privacy concerns the European Union has introduced, with the Global Data Protection Regulation (GDPR), new rules aimed at enforcing the people's rights to personal data protection. The GDPR also gives strong incentives to oISPs to comply. However, today, oISPs can't make their systems GDPR-compliant since they don't have the required technologies. We argue that a new generation of system is mandatory for enabling oISPs to conform to the GDPR. We plan to to design an open source distributed operating system for native implementation of new GDPR rules and ease the programming of compliant cloud-based IoT services. Among the new rules, transparency, right of erasure, and accountability are the most challenging ones to be implemented in IoT environments but could fundamentally increase people's confidence in oISPs. Deployed on individuals' swarms of devices and oISPs' cloud-hosted servers, it will enforce detailed data protection agreements and accountability of oISPs' data processing activities. Ultimately we will show to what extend the new GDPR rules can be implemented for cloud-based IoT services.

3.5. Experimenting with Clouds

Cloud platforms are challenging to evaluate and study with a sound scientific methodology. As with any distributed platform, it is very difficult to gather a global and precise view of the system state. Experiments are not reproducible by default since these systems are shared between several stakeholder. This is even worsen by the fact that microscopic differences in the experimental conditions can lead to drastic changes since typical Cloud applications continuously adapt their behavior to the system conditions.

3.5.1. Experimentation methodologies for clouds

We propose to combine two complementary experimental approaches: direct execution on testbeds such as Grid'5000, that are eminently believable but rather labor intensive, and simulations (using *e.g.* SimGrid) that are much more light-weighted, but requires are careful assessment. One specificity of the Myriads team is that we are working on these experimental methodologies *per se*, raising the standards of *good experiments* in our community.

We plan to make SimGrid widely usable beyond research laboratories, in order to evaluate industrial systems and to teach the future generations of cloud practitioners. This requires to frame the specific concepts of Cloud systems and platforms in actionable interfaces. The challenge is to make the framework both easy to use for simple studies in educational settings while modular and extensible to suit the specific needs of every advanced industrial-class users.

We aim at leveraging the convergence opportunities between methodologies by further bridging simulation and real testbeds. The predictions obtained from the simulator should be validated against some real-world experiments obtained on the target production platform, or on a similar platform. This (in)validation of the predicted results often improves the understanding of the modeled system. On the other side, it may even happen that the measured discrepancies are due to some mis-configuration of the real platform that would have been undetected without this (in)validation study. In that sense, the simulator constitutes a precious tool for the quality assurance of real testbeds such as Grid'5000.

Scientists need more help to make there Cloud experiments fully reproducible, in the sprit of Open Science exemplified by the HAL Open Archive, actively backed by Inria. Users still need practical solutions to archive, share and compare the whole experimental settings, including the raw data production (particularly in the case of real testbeds) and their statistical analysis. This is a long lasting task to which we plan to collaborate through the research communities gathered around the Grid'5000 and SimGrid scientific instruments.

Finally, since correction and performance can constitute contradictory goals, it is particularly important to study them jointly. To that extend, we want to bridge the performance studies, that constitute our main scientific heritage, to correction studies leveraging formal techniques. SimGrid already includes to exhaustively explore the possible executions. We plan to continue this work to ease the use of the relevant formal methods to the experimenter studying Cloud systems.

3.5.2. Use cases

In system research it is important to work on real-world use cases from which we extract requirements inspiring new research directions and with which we can validate the system services and mechanisms we propose. In the framework of our close collaboration with the Data Science Technology department of the LBNL, we will investigate cloud usage for scientific data management. Next-generation scientific discoveries are at the boundaries of datasets, e.g., across multiple science disciplines, institutions and spatial and temporal scales. Today, data integration processes and methods are largely adhoc or manual. A generalized resource infrastructure that integrates knowledge of the data and the processing tasks being performed by the user in the context of the data and resource lifecycle is needed. Clouds provide an important infrastructure platform that can be leveraged by including knowledge for distributed data integration.

PHOENIX Project-Team

3. Research Program

3.1. Design-Driven Software Development

Raising the level of abstraction beyond programming is a very active research topic involving a range of areas, including software engineering, programming languages and formal verification. The challenge is to allow design dimensions of a software system, both functional and non-functional, to be expressed in a high-level way, instead of being encoded with a programming language. Such design dimensions can then be leveraged to verify conformance properties and to generate programming support.

Our research on this topic is to take up this challenge with an approach inspired by programming languages, introducing a full-fledged language for designing software systems and processing design descriptions both for verification and code generation purposes. Our approach is also DSL-inspired in that it defines a conceptual framework to guide software development. Lastly, to make our approach practical to software developers, we introduce a methodology and a suite of tools covering the development life-cycle.

To raise the level of abstraction beyond programming, the key approaches are model-driven engineering and architecture description languages. A number of *architecture description languages* have been proposed; they are either (1) coupled with a programming language (*e.g.,* [37]), providing some level of abstraction above programming, or (2) integrated into a programming language (*e.g.,* [33], [38]), mixing levels of abstraction. Furthermore, these approaches poorly leverage architecture descriptions to support programming, they are crudely integrated into existing development environments, or they are solely used for verification purposes. *Model-driven software development* is another actively researched area. This approach often lacks code generation and verification support. Finally, most (if not all) approaches related to our research goal are *general purpose*; their universal nature provides little, if any, guidance to design a software system. This situation is a major impediment to both reasoning about a design artifact and generating programming support.

3.2. Integrating Non-Functional Concerns into Software Design

Most existing design approaches do not address non-functional concerns. When they do, they do not provide an approach to non-functional concerns that covers the entire development life-cycle. Furthermore, they usually are general purpose, impeding the use of non-functional declarations for verification and code generation. For example, the Architecture Analysis & Design Language (AADL) is a standard dedicated to real-time embedded systems [34]. AADL provides language constructs for the specification of software systems (*e.g.,* component, port) and their deployment on execution platforms (*e.g.,* thread, process, memory). Using AADL, designers specify non-functional aspects by adding properties on language constructs (*e.g.,* the period of a thread) or using language extensions such as the Error Model Annex. [0] The software design concepts of AADL are still rather general purpose and give little guidance to the designer.

Beyond offering a conceptual framework, our language-based approach provides an ideal setting to address non-functional properties (*e.g.,* performance, reliability, security, ...). Specifically, a design language can be enriched with non-functional declarations to pursue three goals: (1) expanding further the type of conformance that can be checked between the design of a software system and its implementation or execution infrastructure, (2) enabling additional programming support and guidance, and (3) leveraging the design declarations to optimize the generated implementation.

We are investigating this idea by extending our design language with non-functional declarations. For example, we have addressed error handling [9], access conflicts to resources [36], quality of service constraints [35], and more recently, data delivery models and parallel computation models for masses of sensors citekaba:hal-01319730.

[0] The Error Model Annex is a standardized AADL extension for the description of errors [39].

Following our approach to paradigm-oriented software development, non-functional declarations are verified at design time, they generate support that guides and constrains programming, they produce a runtime system that preserves invariants and performs efficiently.

3.3. Human-Driven Software Design

Knowledge of the human characteristics (individual, social and organizational) allow the design of complex system and artifacts for increasing their efficacy. In our approach of assistive computing, a main challenge is the integration of facets of Human Factors in order to design technology support adapted to user needs in term of ergonomic properties (acceptability, usability, utility etc) and delivered functionalities (oriented task under user abilities contraints).

We adapt this approach to improve the independent living and self-determination of users with cognitive impairments by developing a variety of orchestration scenarios of networked objects (hardware/software) to provide a pervasive support to their activities. Human factors methodologies are adopted in our approach with the direct purpose the reliability and efficiency of the performance of digital support systems in respect of objectives of health and well-being of the person (monitoring, evaluation, and rehabilitation).

Precisely, our methodologies are based on a closed iterative loop, as described in the figure below :

- Identifying the person needs in a natural situation (*i.e.,* desired but problematic activities) according to Human Factors Models of activity (*i.e.,* environmental constraints; social support networks - caregivers and family; person's abilities)
- Designing environmental support that will assist the users to bypass their cognitive impairment (according to environmental models of cognitive compensatory mechanisms); and then implement this support in terms of technological solutions (scenarios of networked objects, hardware interface, software interface, interaction style, *etc*)
- Empirically evaluating the assistive solution based on human experimentations that includes ergonomic assessments (acceptability, usability, usefulness, *etc*) as well as longitudinal evaluations of use's efficacy in terms of activities performed by the individual, of satisfaction and well-being provided to the individual but also to his/her entourage (family and caregivers).

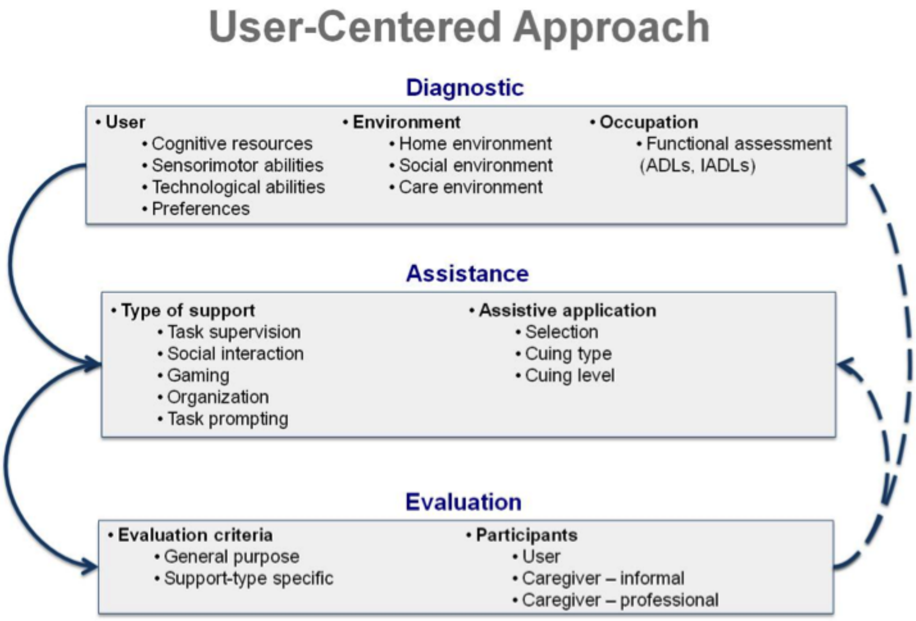


Figure 1. User-Centered Approach

POLARIS Team

3. Research Program

3.1. Sound and Reproducible Experimental Methodology

Participants: Vincent Danjean, Nicolas Gast, Guillaume Huard, Arnaud Legrand, Jean-Marc Vincent.

Experiments in large scale distributed systems are costly, difficult to control and therefore difficult to reproduce. Although many of these digital systems have been built by men, they have reached such a complexity level that we are no longer able to study them like artificial systems and have to deal with the same kind of experimental issues as natural sciences. The development of a sound experimental methodology for the evaluation of resource management solutions is among the most important ways to cope with the growing complexity of computing environments. Although computing environments come with their own specific challenges, we believe such general observation problems should be addressed by borrowing good practices and techniques developed in many other domains of science.

This research theme builds on a transverse activity on *Open science and reproducible research* and is organized into the following two directions: (1) *Experimental design* (2) *Smart monitoring and tracing*. As we will explain in more detail hereafter, these transverse activity and research directions span several research areas and our goal within the POLARIS project is foremost to transfer original ideas from other domains of science to the distributed and high performance computing community.

3.2. Multi-Scale Analysis and Visualization

Participants: Vincent Danjean, Guillaume Huard, Arnaud Legrand, Jean-Marc Vincent, Panayotis Mertikopoulos.

As explained in the previous section, the first difficulty encountered when modeling large scale computer systems is to observe these systems and extract information on the behavior of both the architecture, the middleware, the applications, and the users. The second difficulty is to *visualize* and *analyze* such *multi-level traces to understand how the performance* of the application *can be improved*. While a lot of efforts are put into visualizing scientific data, in comparison little effort have gone into to developing techniques specifically tailored for understanding the behavior of distributed systems. Many visualization tools have been developed by renowned HPC groups since decades (e.g., BSC [87], Jülich and TU Dresden [86], [55], UIUC [74], [90], [77] and ANL [104], Inria Bordeaux [61] and Grenoble [106], ...) but most of these tools build on the classical information visualization mantra [95] that consists in always first presenting an overview of the data, possibly by plotting everything if computing power allows, and then to allow users to zoom and filter, providing details on demand. However in our context, the amount of data comprised in such traces is several orders of magnitude larger than the number of pixels on a screen and displaying even a small fraction of the trace leads to harmful visualization artifacts [82]. Such traces are typically made of events that occur at very different time and space scales, which unfortunately hinders classical approaches. Such visualization tools have focused on easing interaction and navigation in the trace (through gantcharts, intuitive filters, pie charts and kiviats) but they are very difficult to maintain and evolve and they require some significant experience to identify performance bottlenecks.

Therefore many groups have more recently proposed in combination to these tools some techniques to help identifying the structure of the application or regions (applicative, spatial or temporal) of interest. For example, researchers from the SDSC [85] propose some segment matching techniques based on clustering (Euclidean or Manhattan distance) of start and end dates of the segments that enables to reduce the amount of information to display. Researchers from the BSC use clustering, linear regression and Kriging techniques [94], [81], [73] to identify and characterize (in term of performance and resource usage) application phases and present aggregated representations of the trace [93]. Researchers from Jülich and TU Darmstadt have proposed techniques to identify specific communication patterns that incur wait states [101], [48]

3.3. Fast and Faithful Performance Prediction of Very Large Systems

Participants: Vincent Danjean, Bruno Gaujal, Arnaud Legrand, Florence Perronnin, Jean-Marc Vincent.

Evaluating the scalability, robustness, energy consumption and performance of large infrastructures such as exascale platforms and clouds raises severe methodological challenges. The complexity of such platforms mandates empirical evaluation but direct experimentation via an application deployment on a real-world testbed is often limited by the few platforms available at hand and is even sometimes impossible (cost, access, early stages of the infrastructure design, ...). Unlike direct experimentation via an application deployment on a real-world testbed, simulation enables fully repeatable and configurable experiments that can often be conducted quickly for arbitrary hypothetical scenarios. In spite of these promises, current simulation practice is often not conducive to obtaining scientifically sound results. To date, most simulation results in the parallel and distributed computing literature are obtained with simulators that are ad hoc, unavailable, undocumented, and/or no longer maintained. For instance, Naicken et al. [47] point out that out of 125 recent papers they surveyed that study peer-to-peer systems, 52% use simulation and mention a simulator, but 72% of them use a custom simulator. As a result, most published simulation results build on throw-away (short-lived and non validated) simulators that are specifically designed for a particular study, which prevents other researchers from building upon it. There is thus a strong need for recognized simulation frameworks by which simulation results can be reproduced, further analyzed and improved.

The *SimGrid* simulation toolkit [59], whose development is partially supported by POLARIS, is specifically designed for studying large scale distributed computing systems. It has already been successfully used for simulation of grid, volunteer computing, HPC, cloud infrastructures and we have constantly invested on the software quality, the scalability [51] and the validity of the underlying network models [49], [99]. Many simulators of MPI applications have been developed by renowned HPC groups (e.g., at SDSC [97], BSC [45], UIUC [105], Sandia Nat. Lab. [100], ORNL [58] or ETH Zürich [75] for the most prominent ones). Yet, to scale most of them build on restrictive network and application modeling assumptions that make them difficult to extend to more complex architectures and to applications that do not solely build on the MPI API. Furthermore, simplistic modeling assumptions generally prevent to faithfully predict execution times, which limits the use of simulation to indication of gross trends at best. Our goal is to improve the quality of SimGrid to the point where it can be used effectively on a daily basis by practitioners to *reproduce the dynamic of real HPC systems*.

We also develop another simulation software, *PSI* (Perfect SImulator) [63], [56], dedicated to the simulation of very large systems that can be modeled as Markov chains. PSI provides a set of simulation kernels for Markov chains specified by events. It allows one to sample stationary distributions through the Perfect Sampling method (pioneered by Propp and Wilson [88]) or simply to generate trajectories with a forward Monte-Carlo simulation leveraging time parallel simulation (pioneered by Fujimoto [67], Lin and Lazowska [80]). One of the strength of the PSI framework is its expressiveness that allows us to easily study networks with finite and infinite capacity queues [57]. Although PSI already allows to simulate very large and complex systems, our main objective is to push its scalability even further and *improve its capabilities by one or several orders of magnitude*.

3.4. Local Interactions and Transient Analysis in Adaptive Dynamic Systems

Participants: Nicolas Gast, Bruno Gaujal, Florence Perronnin, Jean-Marc Vincent, Panayotis Mertikopoulos.

Many systems can be effectively described by stochastic population models. These systems are composed of a set of n entities interacting together and the resulting stochastic process can be seen as a continuous-time Markov chain with a finite state space. Many numerical techniques exist to study the behavior of Markov chains, to solve stochastic optimal control problems [89] or to perform model-checking [46]. These techniques, however, are limited in their applicability, as they suffer from the *curse of dimensionality*: the state-space grows exponentially with n.

This results in the need for approximation techniques. Mean field analysis offers a viable, and often very accurate, solution for large n. The basic idea of the mean field approximation is to count the number of entities that are in a given state. Hence, the fluctuations due to stochasticity become negligible as the number of entities grows. For large n, the system becomes essentially deterministic. This approximation has been originally developed in statistical mechanics for vary large systems composed of more than 10^{20} particles (called entities here). More recently, it has been claimed that, under some conditions, this approximation can be successfully used for stochastic systems composed of a few tens of entities. The claim is supported by various convergence results [68], [78], [103], and has been successfully applied in various domains: wireless networks [50], computer-based systems [71], [84], [98], epidemic or rumour propagation [60], [76] and bike-sharing systems [64]. It is also used to develop distributed control strategies [102], [83] or to construct approximate solutions of stochastic model checking problems [52], [53], [54].

Within the POLARIS project, we will continue developing both the theory behind these approximation techniques and their applications. Typically, these techniques require a homogeneous population of objects where the dynamics of the entities depend only on their state (the state space of each object must not scale with n the number of objects) but neither on their identity nor on their spatial location. Continuing our work in [68], we would like to be able to handle heterogeneous or uncertain dynamics. Typical applications are caching mechanisms [71] or bike-sharing systems [65]. A second point of interest is the use of mean field or large deviation asymptotics to compute the time between two regimes [92] or to reach an equilibrium state. Last, mean-field methods are mostly descriptive and are used to analyse the performance of a given system. We wish to extend their use to solve optimal control problems. In particular, we would like to implement numerical algorithms that use the framework that we developed in [69] to build distributed control algorithms [62] and optimal pricing mechanisms [70].

3.5. Distributed Learning in Games and Online Optimization

Participants: Nicolas Gast, Bruno Gaujal, Arnaud Legrand, Panayotis Mertikopoulos.

Game theory is a thriving interdisciplinary field that studies the interactions between competing optimizing agents, be they humans, firms, bacteria, or computers. As such, game-theoretic models have met with remarkable success when applied to complex systems consisting of interdependent components with vastly different (and often conflicting) objectives – ranging from latency minimization in packet-switched networks to throughput maximization and power control in mobile wireless networks.

In the context of large-scale, decentralized systems (the core focus of the POLARIS project), it is more relevant to take an inductive, "bottom-up" approach to game theory, because the components of a large system cannot be assumed to perform the numerical calculations required to solve a very-large-scale optimization problem. In view of this, POLARIS' overarching objective in this area is to *develop novel algorithmic frameworks that offer robust performance guarantees when employed by all interacting decision-makers.*

A key challenge here is that most of the literature on learning in games has focused on *static* games with a *finite number of actions* per player [66], [91]. While relatively tractable, such games are ill-suited to practical applications where players pick an action from a continuous space or when their payoff functions evolve over time – this being typically the case in our target applications (e.g., routing in packet-switched networks or energy-efficient throughput maximization in wireless). On the other hand, the framework of online convex optimization typically provides worst-case performance bounds on the learner's *regret* that the agents can attain irrespectively of how their environment varies over time. However, if the agents' environment is determined chiefly by their interactions these bounds are fairly loose, so more sophisticated convergence criteria should be applied.

From an algorithmic standpoint, a further challenge occurs when players can only observe their own payoffs (or a perturbed version thereof). In this bandit-like setting regret-matching or trial-and-error procedures guarantee convergence to an equilibrium in a weak sense in certain classes of games. However, these results apply exclusively to static, finite games: learning in games with continuous action spaces and/or nonlinear payoff functions cannot be studied within this framework. Furthermore, even in the case of finite games, the complexity of the algorithms described above is not known, so it is impossible to decide a priori which algorithmic scheme can be applied to which application.

RAP Project-Team

3. Research Program

3.1. Scaling of Markov Processes

The growing complexity of communication networks makes it more difficult to apply classical mathematical methods. For a one/two-dimensional Markov process describing the evolution of some network, it is sometimes possible to write down the equilibrium equations and to solve them. The key idea to overcome these difficulties is to consider the system in limit regimes. This list of possible renormalization procedures is, of course, not exhaustive. The advantages of these methods lie in their flexibility to various situations and to the interesting theoretical problems they raised.

A fluid limit scaling is a particularly important means to scale a Markov process. It is related to the first order behavior of the process and, roughly speaking, amounts to a functional law of large numbers for the system considered.

A fluid limit keeps the main characteristics of the initial stochastic process while some second order stochastic fluctuations disappear. In “good” cases, a fluid limit is a deterministic function, obtained as the solution of some ordinary differential equation. As can be expected, the general situation is somewhat more complicated. These ideas of rescaling stochastic processes have emerged recently in the analysis of stochastic networks, to study their ergodicity properties in particular.

3.2. Design and Analysis of Algorithms

Data Structures, Stochastic Algorithms

The general goal of the research in this domain is of designing algorithms to analyze and control the traffic of communication networks. The team is currently involved in the design of algorithms to allocate bandwidth in optical networks and also to allocate resources in large distributed networks. See the corresponding sections below.

The team also pursues analysis of algorithms and data structures in the spirit of the former Algorithms team. The team is especially interested in the ubiquitous divide-and-conquer paradigm and its applications to the design of search trees, and stable collision resolution protocols.

3.3. Structure of random networks

This line of research aims at understanding the global structure of stochastic networks (connectivity, magnitude of distances, etc) via models of random graphs. It consists of two complementary foundational and applied aspects of connectivity.

RANDOM GRAPHS, STATISTICAL PHYSICS AND COMBINATORIAL OPTIMIZATION. The connectivity of usual models for networks based on random graphs models (Erdős–Rényi and random geometric graphs) may be tuned by adjusting the average degree. There is a *phase transition* as the average degree approaches one, a *giant* connected component containing a positive proportion of the nodes suddenly appears. The phase of practical interest is the *supercritical* one, when there is at least a giant component, while the theoretical interest lies at the *critical phase*, the break-point just before it appears.

At the critical point there is not yet a macroscopic component and the network consists of a large number of connected component at the mesoscopic scale. From a theoretical point of view, this phase is most interesting since the structure of the clusters there is expected (heuristically) to be *universal*. Understanding this phase and its universality is a great challenge that would impact the knowledge of phase transitions in all high-dimensional models of *statistical physics* and *combinatorial optimization*.

RANDOM GEOMETRIC GRAPHS AND WIRELESS NETWORKS. The level of connection of the network is of course crucial, but the *scalability* imposes that the underlying graph also be *sparse*: trade offs must be made, which required a fine evaluation of the costs/benefits. Various direct and indirect measures of connectivity are crucial to these choices: What is the size of the overwhelming connected component? When does complete connectivity occur? What is the order of magnitude of distances? Are paths to a target easy to find using only local information? Are there simple broadcasting algorithms? Can one put an end to viral infections? How much time for a random crawler to see most of the network?

NAVIGATION AND POINT LOCATION IN RANDOM MESHES. Other applications which are less directly related to networks include the design of improved navigation or point location algorithms in geometric meshes such as the Delaunay triangulation build from random point sets. There the graph model is essentially fixed, but the constraints it imposes raise a number of challenging problems. The aim is to prove performance guarantees for these algorithms which are used in most manipulations of the meshes.

REGAL Project-Team

3. Research Program

3.1. Research rationale

The research of Regal addresses both theoretical and practical issues of *Computer Systems*, i.e., its goal is a dual expertise in theoretical and experimental research. Our approach is a “virtuous cycle” of algorithm design triggered by issues with real systems, which we prove correct and evaluate theoretically, and then eventually implement and test experimentally.

Regal’s major challenges comprise communication, sharing of information, and correct execution in large-scale and/or highly dynamic computer systems. While Regal’s historically focused in static distributed systems, since some years ago we have covered a larger spectrum of distributed computer systems: multicore computers, clusters, mobile networks, peer-to-peer systems, cloud computing systems, and other communicating entities such as swarms of robots. This holistic approach allows the handling of related problems at different levels. Among such problems we can highlight communication between cores, consensus, fault detection, scalability, search and diffusion of information, allocation resource, replication and consistency of shared data, dynamic content distribution, and multi-core concurrent algorithms.

Computer Systems is a rapidly evolving domain, with strong interactions with industry and modern computer systems, which are increasingly distributed. Ensuring persistence, availability, and consistency of data in a distributed setting is a major requirement: the system must remain correct despite slow networks, disconnection, crashes, failures, churn, and attacks. Easiness of use, performance, and efficiency are equally fundamental. However, these requirements are somewhat conflicting, and there are many algorithmic and engineering trade-offs, which often depend on specific workloads or usage scenarios. At the same time, years of research in distributed systems are now coming to fruition, and are being used by millions of users of web systems, peer-to-peer systems, gaming and social applications, or cloud computing. These new usages bring new challenges of extreme scalability and adaptation to dynamically-changing conditions, where knowledge of the system state might only be partial and incomplete. Therefore, the scientific challenges of the distributed computing systems listed above are subject to additional trade-offs which include scalability, fault tolerance, dynamics, and virtualization of physical infrastructure. Algorithms designed for traditional distributed systems, such as resource allocation, data storage and placement, and concurrent access to shared data, need to be redefined or revisited in order to work properly under the constraints of these new environments.

In in particular, Regal focuses on three key challenges:

- the adaptation of algorithms to the new dynamics of distributed systems;
- data management on extreme large configurations;
- the adaptation of execution support to new multi-core architectures.

We should emphasize that these challenges are complementary: the two first challenges aim at building new distributed algorithms and strategies for large and dynamic distributed configurations whereas the last one focusses on the scalability of internal OS mechanisms.

RMOD Project-Team

3. Research Program

3.1. Software Reengineering

Strong coupling among the parts of an application severely hampers its evolution. Therefore, it is crucial to answer the following questions: How to support the substitution of certain parts while limiting the impact on others? How to identify reusable parts? How to modularize an object-oriented application?

Having good classes does not imply a good application layering, absence of cycles between packages and reuse of well-identified parts. Which notion of cohesion makes sense in presence of late-binding and programming frameworks? Indeed, frameworks define a context that can be extended by subclassing or composition: in this case, packages can have a low cohesion without being a problem for evolution. How to obtain algorithms that can be used on real cases? Which criteria should be selected for a given remodularization?

To help us answer these questions, we work on enriching Moose, our reengineering environment, with a new set of analyses [45], [44]. We decompose our approach in three main and potentially overlapping steps:

1. Tools for understanding applications,
2. Remodularization analyses,
3. Software Quality.

3.1.1. Tools for understanding applications

Context and Problems. We are studying the problems raised by the understanding of applications at a larger level of granularity such as packages or modules. We want to develop a set of conceptual tools to support this understanding.

Some approaches based on Formal Concept Analysis (FCA) [75] show that such an analysis can be used to identify modules. However the presented examples are too small and not representative of real code.

Research Agenda.

FCA provides an important approach in software reengineering for software understanding, design anomalies detection and correction, but it suffers from two problems: (i) it produces lattices that must be interpreted by the user according to his/her understanding of the technique and different elements of the graph; and, (ii) the lattice can rapidly become so big that one is overwhelmed by the mass of information and possibilities [34]. We look for solutions to help people putting FCA to real use.

3.1.2. Remodularization analyses

Context and Problems. It is a well-known practice to layer applications with bottom layers being more stable than top layers [61]. Until now, few works have attempted to identify layers in practice: Mudpie [77] is a first cut at identifying cycles between packages as well as package groups potentially representing layers. DSM (dependency structure matrix) [76], [69] seems to be adapted for such a task but there is no serious empirical experience that validates this claim. From the side of remodularization algorithms, many were defined for procedural languages [57]. However, object-oriented programming languages bring some specific problems linked with late-binding and the fact that a package does not have to be systematically cohesive since it can be an extension of another one [78], [48].

As we are designing and evaluating algorithms and analyses to remodularize applications, we also need a way to understand and assess the results we are obtaining.

Research Agenda. We work on the following items:

Layer identification. We propose an approach to identify layers based on a semi-automatic classification of package and class interrelationships that they contain. However, taking into account the wish or knowledge of the designer or maintainer should be supported.

Cohesion Metric Assessment. We are building a validation framework for cohesion/coupling metrics to determine whether they actually measure what they promise to. We are also compiling a number of traditional metrics for cohesion and coupling quality metrics to evaluate their relevance in a software quality setting.

3.1.3. Software Quality

Research Agenda. Since software quality is fuzzy by definition and a lot of parameters should be taken into account we consider that defining precisely a unique notion of software quality is definitively a Grail in the realm of software engineering. The question is still relevant and important. We work on the two following items:

Quality models. We studied existing quality models and the different options to combine indicators — often, software quality models happily combine metrics, but at the price of losing the explicit relationships between the indicator contributions. There is a need to combine the results of one metric over all the software components of a system, and there is also the need to combine different metric results for any software component. Different combination methods are possible that can give very different results. It is therefore important to understand the characteristics of each method.

Bug prevention. Another aspect of software quality is validating or monitoring the source code to avoid the emergence of well known sources of errors and bugs. We work on how to best identify such common errors, by trying to identify earlier markers of possible errors, or by helping identifying common errors that programmers did in the past.

3.2. Language Constructs for Modular Design

While the previous axis focuses on how to help remodularizing existing software, this second research axis aims at providing new language constructs to build more flexible and recomposable software. We will build on our work on traits [73], [46] and classboxes [35] but also start to work on new areas such as isolation in dynamic languages. We will work on the following points: (1) Traits and (2) Modularization as a support for isolation.

3.2.1. Traits-based program reuse

Context and Problems. Inheritance is well-known and accepted as a mechanism for reuse in object-oriented languages. Unfortunately, due to the coarse granularity of inheritance, it may be difficult to decompose an application into an optimal class hierarchy that maximizes software reuse. Existing schemes based on single inheritance, multiple inheritance, or mixins, all pose numerous problems for reuse.

To overcome these problems, we designed a new composition mechanism called Traits [73], [46]. Traits are pure units of behavior that can be composed to form classes or other traits. The trait composition mechanism is an alternative to multiple or mixin inheritance in which the composer has full control over the trait composition. The result enables more reuse than single inheritance without introducing the drawbacks of multiple or mixin inheritance. Several extensions of the model have been proposed [43], [65], [36], [47] and several type systems were defined [49], [74], [66], [59].

Traits are reusable building blocks that can be explicitly composed to share methods across unrelated class hierarchies. In their original form, traits do not contain state and cannot express visibility control for methods. Two extensions, stateful traits and freezable traits, have been proposed to overcome these limitations. However, these extensions are complex both to use for software developers and to implement for language designers.

Research Agenda: Towards a pure trait language. We plan distinct actions: (1) a large application of traits, (2) assessment of the existing trait models and (3) bootstrapping a pure trait language.

- To evaluate the expressiveness of traits, some hierarchies were refactored, showing code reuse [38]. However, such large refactorings, while valuable, may not exhibit all possible composition problems, since the hierarchies were previously expressed using single inheritance and following certain patterns. We want to redesign from scratch the collection library of Smalltalk (or part of it). Such a redesign should on the one hand demonstrate the added value of traits on a real large and redesigned library and on the other hand foster new ideas for the bootstrapping of a pure trait-based language.

  In particular we want to reconsider the different models proposed (stateless [46], stateful [37], and freezable [47]) and their operators. We will compare these models by (1) implementing a trait-based collection hierarchy, (2) analyzing several existing applications that exhibit the need for traits. Traits may be flattened [64]. This is a fundamental property that confers to traits their simplicity and expressiveness over Eiffel's multiple inheritance. Keeping these aspects is one of our priority in forthcoming enhancements of traits.
- Alternative trait models. This work revisits the problem of adding state and visibility control to traits. Rather than extending the original trait model with additional operations, we use a fundamentally different approach by allowing traits to be lexically nested within other modules. This enables traits to express (shared) state and visibility control by hiding variables or methods in their lexical scope. Although the traits' "flattening property" no longer holds when they can be lexically nested, the combination of traits with lexical nesting results in a simple and more expressive trait model. We formally specify the operational semantics of this combination. Lexically nested traits are fully implemented in AmbientTalk, where they are used among others in the development of a Morphic-like UI framework.
- We want to evaluate how inheritance can be replaced by traits to form a new object model. For this purpose we will design a minimal reflective kernel, inspired first from ObjVlisp [42] then from Smalltalk [52].

3.2.2. Reconciling Dynamic Languages and Isolation

Context and Problems. More and more applications require dynamic behavior such as modification of their own execution (often implemented using reflective features [56]). For example, F-script allows one to script Cocoa Mac-OS X applications and Lua is used in Adobe Photoshop. Now in addition more and more applications are updated on the fly, potentially loading untrusted or broken code, which may be problematic for the system if the application is not properly isolated. Bytecode checking and static code analysis are used to enable isolation, but such approaches do not really work in presence of dynamic languages and reflective features. Therefore there is a tension between the need for flexibility and isolation.

Research Agenda: Isolation in dynamic and reflective languages. To solve this tension, we will work on *Sure*, a language where isolation is provided by construction: as an example, if the language does not offer field access and its reflective facilities are controlled, then the possibility to access and modify private data is controlled. In this context, layering and modularizing the meta-level [39], as well as controlling the access to reflective features [40], [41] are important challenges. We plan to:

- Study the isolation abstractions available in erights (http://www.erights.org) [63], [62], and Java's class loader strategies [58], [53].
- Categorize the different reflective features of languages such as CLOS [55], Python and Smalltalk [67] and identify suitable isolation mechanisms and infrastructure [50].
- Assess different isolation models (access rights, capabilities [68]...) and identify the ones adapted to our context as well as different access and right propagation.
- Define a language based on
  - the decomposition and restructuring of the reflective features [39],

- the use of encapsulation policies as a basis to restrict the interfaces of the controlled objects [72],
- the definition of method modifiers to support controlling encapsulation in the context of dynamic languages.

An open question is whether, instead of providing restricted interfaces, we could use traits to grant additional behavior to specific instances: without trait application, the instances would only exhibit default public behavior, but with additional traits applied, the instances would get extra behavior. We will develop *Sure*, a modular extension of the reflective kernel of Smalltalk (since it is one of the languages offering the largest set of reflective features such as pointer swapping, class changing, class definition...) [67].

ROMA Project-Team

3. Research Program

3.1. Algorithms for probabilistic environments

There are two main research directions under this research theme. In the first one, we consider the problem of the efficient execution of applications in a failure-prone environment. Here, probability distributions are used to describe the potential behavior of computing platforms, namely when hardware components are subject to faults. In the second research direction, probability distributions are used to describe the characteristics and behavior of applications.

3.1.1. Application resilience

An application is resilient if it can successfully produce a correct result in spite of potential faults in the underlying system. Application resilience can involve a broad range of techniques, including fault prediction, error detection, error containment, error correction, checkpointing, replication, migration, recovery, etc. Faults are quite frequent in the most powerful existing supercomputers. The Jaguar platform, which ranked third in the TOP 500 list in November 2011 [59], had an average of 2.33 faults per day during the period from August 2008 to February 2010 [83]. The mean-time between faults of a platform is inversely proportional to its number of components. Progresses will certainly be made in the coming years with respect to the reliability of individual components. However, designing and building high-reliability hardware components is far more expensive than using lower reliability top-of-the-shelf components. Furthermore, low-power components may not be available with high-reliability. Therefore, it is feared that the progresses in reliability will far from compensate the steady projected increase of the number of components in the largest supercomputers. Already, application failures have a huge computational cost. In 2008, the DARPA white paper on "System resilience at extreme scale" [58] stated that high-end systems wasted 20% of their computing capacity on application failure and recovery.

In such a context, any application using a significant fraction of a supercomputer and running for a significant amount of time will have to use some fault-tolerance solution. It would indeed be unacceptable for an application failure to destroy centuries of CPU-time (some of the simulations run on the Blue Waters platform consumed more than 2,700 years of core computing time [54] and lasted over 60 hours; the most time-consuming simulations of the US Department of Energy (DoE) run for weeks to months on the most powerful existing platforms [57]).

Our research on resilience follows two different directions. On the one hand we design new resilience solutions, either generic fault-tolerance solutions or algorithm-based solutions. On the other hand we model and theoretically analyze the performance of existing and future solutions, in order to tune their usage and help determine which solution to use in which context.

3.1.2. Scheduling strategies for applications with a probabilistic behavior

Static scheduling algorithms are algorithms where all decisions are taken before the start of the application execution. On the contrary, in non-static algorithms, decisions may depend on events that happen during the execution. Static scheduling algorithms are known to be superior to dynamic and system-oriented approaches in stable frameworks [65], [71], [72], [82], that is, when all characteristics of platforms and applications are perfectly known, known a priori, and do not evolve during the application execution. In practice, the prediction of application characteristics may be approximative or completely infeasible. For instance, the amount of computations and of communications required to solve a given problem in parallel may strongly depend on some input data that are hard to analyze (this is for instance the case when solving linear systems using full pivoting).

We plan to consider applications whose characteristics change dynamically and are subject to uncertainties. In order to benefit nonetheless from the power of static approaches, we plan to model application uncertainties and variations through probabilistic models, and to design for these applications scheduling strategies that are either static, or partially static and partially dynamic.

3.2. Platform-aware scheduling strategies

In this theme, we study and design scheduling strategies, focusing either on energy consumption or on memory behavior. In other words, when designing and evaluating these strategies, we do not limit our view to the most classical platform characteristics, that is, the computing speed of cores and accelerators, and the bandwidth of communication links.

In most existing studies, a single optimization objective is considered, and the target is some sort of absolute performance. For instance, most optimization problems aim at the minimization of the overall execution time of the application considered. Such an approach can lead to a very significant waste of resources, because it does not take into account any notion of efficiency nor of yield. For instance, it may not be meaningful to use twice as many resources just to decrease by 10% the execution time. In all our work, we plan to look only for algorithmic solutions that make a "clever" usage of resources. However, looking for the solution that optimizes a metric such as the efficiency, the energy consumption, or the memory-peak minimization, is doomed for the type of applications we consider. Indeed, in most cases, any optimal solution for such a metric is a sequential solution, and sequential solutions have prohibitive execution times. Therefore, it becomes mandatory to consider multi-criteria approaches where one looks for trade-offs between some user-oriented metrics that are typically related to notions of Quality of Service—execution time, response time, stretch, throughput, latency, reliability, etc.—and some system-oriented metrics that guarantee that resources are not wasted. In general, we will not look for the Pareto curve, that is, the set of all dominating solutions for the considered metrics. Instead, we will rather look for solutions that minimize some given objective while satisfying some bounds, or "budgets", on all the other objectives.

3.2.1. Energy-aware algorithms

Energy-aware scheduling has proven an important issue in the past decade, both for economical and environmental reasons. Energy issues are obvious for battery-powered systems. They are now also important for traditional computer systems. Indeed, the design specifications of any new computing platform now always include an upper bound on energy consumption. Furthermore, the energy bill of a supercomputer may represent a significant share of its cost over its lifespan.

Technically, a processor running at speed s dissipates s^α watts per unit of time with $2 \leq \alpha \leq 3$ [63], [64], [69]; hence, it consumes $s^\alpha \times d$ joules when operated during d units of time. Therefore, energy consumption can be reduced by using speed scaling techniques. However it was shown in [84] that reducing the speed of a processor increases the rate of transient faults in the system. The probability of faults increases exponentially, and this probability cannot be neglected in large-scale computing [80]. In order to make up for the loss in *reliability* due to the energy efficiency, different models have been proposed for fault tolerance: (i) *re-execution* consists in re-executing a task that does not meet the reliability constraint [84]; (ii) *replication* consists in executing the same task on several processors simultaneously, in order to meet the reliability constraints [62]; and (iii) *checkpointing* consists in "saving" the work done at some certain instants, hence reducing the amount of work lost when a failure occurs [79].

Energy issues must be taken into account at all levels, including the algorithm-design level. We plan to both evaluate the energy consumption of existing algorithms and to design new algorithms that minimize energy consumption using tools such as resource selection, dynamic frequency and voltage scaling, or powering-down of hardware components.

3.2.2. Memory-aware algorithms

For many years, the bandwidth between memories and processors has increased more slowly than the computing power of processors, and the latency of memory accesses has been improved at an even slower pace. Therefore, in the time needed for a processor to perform a floating point operation, the amount of data transferred between the memory and the processor has been decreasing with each passing year. The risk is for an application to reach a point where the time needed to solve a problem is no longer dictated by the processor computing power but by the memory characteristics, comparable to the *memory wall* that limits CPU performance. In such a case, processors would be greatly under-utilized, and a large part of the computing power of the platform would be wasted. Moreover, with the advent of multicore processors, the amount of memory per core has started to stagnate, if not to decrease. This is especially harmful to memory intensive applications. The problems related to the sizes and the bandwidths of memories are further exacerbated on modern computing platforms because of their deep and highly heterogeneous hierarchies. Such a hierarchy can extend from core private caches to shared memory within a CPU, to disk storage and even tape-based storage systems, like in the Blue Waters supercomputer [55]. It may also be the case that heterogeneous cores are used (such as hybrid CPU and GPU computing), and that each of them has a limited memory.

Because of these trends, it is becoming more and more important to precisely take memory constraints into account when designing algorithms. One must not only take care of the amount of memory required to run an algorithm, but also of the way this memory is accessed. Indeed, in some cases, rather than to minimize the amount of memory required to solve the given problem, one will have to maximize data reuse and, especially, to minimize the amount of data transferred between the different levels of the memory hierarchy (minimization of the volume of memory inputs-outputs). This is, for instance, the case when a problem cannot be solved by just using the in-core memory and that any solution must be out-of-core, that is, must use disks as storage for temporary data.

It is worth noting that the cost of moving data has lead to the development of so called "communication-avoiding algorithms" [76]. Our approach is orthogonal to these efforts: in communication-avoiding algorithms, the application is modified, in particular some redundant work is done, in order to get rid of some communication operations, whereas in our approach, we do not modify the application, which is provided as a task graph, but we minimize the needed memory peak only by carefully scheduling tasks.

3.3. High-performance computing and linear algebra

Our work on high-performance computing and linear algebra is organized along three research directions. The first direction is devoted to direct solvers of sparse linear systems. The second direction is devoted to combinatorial scientific computing, that is, the design of combinatorial algorithms and tools that solve problems encountered in some of the other research themes, like the problems faced in the preprocessing phases of sparse direct solvers. The last direction deals with the adaptation of classical dense linear algebra kernels to the architecture of future computing platforms.

3.3.1. Direct solvers for sparse linear systems

The solution of sparse systems of linear equations (symmetric or unsymmetric, often with an irregular structure, from a few hundred thousand to a few hundred million equations) is at the heart of many scientific applications arising in domains such as geophysics, structural mechanics, chemistry, electromagnetism, numerical optimization, or computational fluid dynamics, to cite a few. The importance and diversity of applications are a main motivation to pursue research on sparse linear solvers. Because of this wide range of applications, any significant progress on solvers will have a significant impact in the world of simulation. Research on sparse direct solvers in general is very active for the following main reasons:

- many applications fields require large-scale simulations that are still too big or too complicated with respect to today's solution methods;
- the current evolution of architectures with massive, hierarchical, multicore parallelism imposes to overhaul all existing solutions, which represents a major challenge for algorithm and software development;
- the evolution of numerical needs and types of simulations increase the importance, frequency, and size of certain classes of matrices, which may benefit from a specialized processing (rather than resort to a generic one).

Our research in the field is strongly related to the software package MUMPS (see Section 6.1). MUMPS is both an experimental platform for academics in the field of sparse linear algebra, and a software package that is widely used in both academia and industry. The software package MUMPS enables us to (i) confront our research to the real world, (ii) develop contacts and collaborations, and (iii) receive continuous feedback from real-life applications, which is extremely critical to validate our research work. The feedback from a large user community also enables us to direct our long-term objectives towards meaningful directions.

In this context, we aim at designing parallel sparse direct methods that will scale to large modern platforms, and that are able to answer new challenges arising from applications, both efficiently—from a resource consumption point of view—and accurately—from a numerical point of view. For that, and even with increasing parallelism, we do not want to sacrifice in any manner numerical stability, based on threshold partial pivoting, one of the main originalities of our approach (our "trademark") in the context of direct solvers for distributed-memory computers; although this makes the parallelization more complicated, applying the same pivoting strategy as in the serial case ensures numerical robustness of our approach, which we generally measure in terms of sparse backward error. In order to solve the hard problems resulting from the always-increasing demands in simulations, special attention must also necessarily be paid to memory usage (and not only execution time). This requires specific algorithmic choices and scheduling techniques. From a complementary point of view, it is also necessary to be aware of the functionality requirements from the applications and from the users, so that robust solutions can be proposed for a wide range of applications.

Among direct methods, we rely on the multifrontal method [73], [74], [78]. This method usually exhibits a good data locality and hence is efficient in cache-based systems. The task graph associated with the multifrontal method is in the form of a tree whose characteristics should be exploited in a parallel implementation.

Our work is organized along two main research directions. In the first one we aim at efficiently addressing new architectures that include massive, hierarchical parallelism. In the second one, we aim at reducing the running time complexity and the memory requirements of direct solvers, while controlling accuracy.

3.3.2. Combinatorial scientific computing

Combinatorial scientific computing (CSC) is a recently coined term (circa 2002) for interdisciplinary research at the intersection of discrete mathematics, computer science, and scientific computing. In particular, it refers to the development, application, and analysis of combinatorial algorithms to enable scientific computing applications. CSC's deepest roots are in the realm of direct methods for solving sparse linear systems of equations where graph theoretical models have been central to the exploitation of sparsity, since the 1960s. The general approach is to identify performance issues in a scientific computing problem, such as memory use, parallel speed up, and/or the rate of convergence of a method, and to develop combinatorial algorithms and models to tackle those issues.

Our target scientific computing applications are (i) the preprocessing phases of direct methods (in particular MUMPS), iterative methods, and hybrid methods for solving linear systems of equations, and tensor decomposition algorithms; and (ii) the mapping of tasks (mostly the sub-tasks of the mentioned solvers) onto modern computing platforms. We focus on the development and use of graph and hypergraph models, and related tools such as hypergraph partitioning algorithms, to solve problems of load balancing and task mapping. We also focus on bipartite graph matching and vertex ordering methods for reducing the memory overhead and computational requirements of solvers. Although we direct our attention on these models and algorithms through the lens of linear system solvers, our solutions are general enough to be applied to some other resource optimization problems.

3.3.3. Dense linear algebra on post-petascale multicore platforms

The quest for efficient, yet portable, implementations of dense linear algebra kernels (QR, LU, Cholesky) has never stopped, fueled in part by each new technological evolution. First, the LAPACK library [67] relied on BLAS level 3 kernels (Basic Linear Algebra Subroutines) that enable to fully harness the computing power of a single CPU. Then the SCALAPACK library [66] built upon LAPACK to provide a coarse-grain parallel version, where processors operate on large block-column panels. Inter-processor communications occur through highly tuned MPI send and receive primitives. The advent of multi-core processors has led to a major modification in these algorithms [68], [81], [77]. Each processor runs several threads in parallel to keep all cores within that processor busy. Tiled versions of the algorithms have thus been designed: dividing large block-column panels into several tiles allows for a decrease in the granularity down to a level where many smaller-size tasks are spawned. In the current panel, the diagonal tile is used to eliminate all the lower tiles in the panel. Because the factorization of the whole panel is now broken into the elimination of several tiles, the update operations can also be partitioned at the tile level, which generates many tasks to feed all cores.

The number of cores per processor will keep increasing in the following years. It is projected that high-end processors will include at least a few hundreds of cores. This evolution will require to design new versions of libraries. Indeed, existing libraries rely on a static distribution of the work: before the beginning of the execution of a kernel, the location and time of the execution of all of its component is decided. In theory, static solutions enable to precisely optimize executions, by taking parameters like data locality into account. At run time, these solutions proceed at the pace of the slowest of the cores, and they thus require a perfect load-balancing. With a few hundreds, if not a thousand, cores per processor, some tiny differences between the computing times on the different cores ("jitter") are unavoidable and irremediably condemn purely static solutions. Moreover, the increase in the number of cores per processor once again mandates to increase the number of tasks that can be executed in parallel.

We study solutions that are part-static part-dynamic, because such solutions have been shown to outperform purely dynamic ones [70]. On the one hand, the distribution of work among the different nodes will still be statically defined. On the other hand, the mapping and the scheduling of tasks inside a processor will be dynamically defined. The main difficulty when building such a solution will be to design lightweight dynamic schedulers that are able to guarantee both an excellent load-balancing and a very efficient use of data locality.

3.4. Compilers, code optimization and high-level synthesis for FPGA

Christophe Alias and Laure Gonnord asked to join the ROMA team temporarily, starting from September 2015. This was accepted by the team and by Inria. The text below describes their research domain. The results that they have achieved in 2016 are included in this report.

The advent of parallelism in supercomputers, in embedded systems (smartphones, plane controllers), and in more classical end-user computers increases the need for high-level code optimization and improved compilers. Being able to deal with the complexity of the upcoming software and hardware while keeping energy consumption at a reasonnable level is one of the main challenges cited in the Hipeac Roadmap which among others cites the two major issues :

- Enhance the efficiency of the design of embedded systems, and especially the design of optimized specialized hardware.
- Invent techniques to "expose data movement in applications and optimize them at runtime and compile time and to investigate communication-optimized algorithms".

In particular, the rise of embedded systems and high performance computers in the last decade has generated new problems in code optimization, with strong consequences on the research area. The main challenge is to take advantage of the characteristics of the specific hardware (generic hardware, or hardware accelerators). The long-term objective is to provide solutions for the end-user developers to use at their best the huge opportunities of these emerging platforms.

3.4.1. Compiler algorithms for irregular applications

In the last decades, several frameworks has emerged to design efficient compiler algorithms. The efficiency of all the optimizations performed in compilers strongly relies on performant *static analyses* and *intermediate representations*. Among these representations, the polyhedral model [75] focus on regular programs, whose execution trace is predictable statically. The program and the data accessed are represented with a single mathematical object endowed with powerful algorithmic techniques for reasoning about it. Unfortunately, most of the algorithms used in scientific computing do not fit totally in this category.

We plan to explore the extensions of these techniques to handle irregular programs with while loops and complex data structures (such as trees, and lists). This raises many issues. We cannot represent finitely all the possible executions traces. Which approximation/representation to choose? Then, how to adapt existing techniques on approximated traces while preserving the correctness? To address these issues, we plan to incorporate new ideas coming from the abstract interpretation community: control flow, approximations, and also shape analysis; and from the termination community: rewriting is one of the major techniques that are able to handle complex data structures and also recursive programs.

3.4.2. High-level synthesis for FPGA

Energy consumption bounds the performance of supercomputers since the end of Dennard scaling. Hence, reducing the electrical energy spent in a computation is the major challenge raised by Exaflop computing. Novel hardware, software, compilers and operating systems must be designed to increase the energy efficiency (in flops/watt) of data manipulation and computation itself. In the last decade, many specialized hardware accelerators (Xeon Phi, GPGPU) has emerged to overcome the limitations of mainstream processors, by trading the genericity for energy efficiency. However, the best supercomputers can only reach 8 Gflops/watt [61], which is far less than the 50 Gflops/watt required by an Exaflop supercomputer. An extreme solution would be to trade all the genericity by using specialized circuits. However such circuits (application specific integrated circuits, ASIC) are usually too expensive for the HPC market and lacks of flexibility. Once printed, an ASIC cannot be modified. Any algorithm update (or bug fix) would be impossible, which clearly not realistic.

Recently, reconfigurable circuits (Field Programmable Gate Arrays, FPGA) has appeared as a credible alternative for Exaflop computing. Major companies (including Intel, Google, Facebook and Microsoft) show a growing interest to FPGA and promising results has been obtained. For instance, in 2015, Microsoft reaches 40 Gflop/watts on a data-center deep learning algorithm mapped on Intel/Altera Arria 10 FPGAs. We believe that FPGA will become the new building block for HPC and Big Data systems. Unfortunately, programming an FPGA is still a big challenge: the application must be defined at circuit level and use properly the logic cells. Hence, there is a strong need for a compiler technology able to *map complex applications specified in a high-level language*. This compiler technology is usually refered as high-level synthesis (HLS).

We plan to investigate how to extend the models and the algorithms developed by the HPC community to map automatically a complex application to an FPGA. This raises many issues. How to schedule/allocate the computations and the data on the FPGA in order to reduce the data transfers while keeping a high throughput? How to use optimally the resources of the FPGA while keeping a low critical path? To address these issues, we plan to develop novel execution models based on process networks and to extend/cross-fertilize the algorithms developed in both HPC and high-level synthesis communities. The purpose of the XtremLogic start-up company, co-founded by Christophe Alias and Alexandru Plesco is to transfer the results of this research to an industrial level compiler.

SOCRATE Project-Team

3. Research Program

3.1. Research Axes

In order to keep young researchers in an environment close to their background, we have structured the team along the three research axes related to the three main scientific domains spanned by Socrate. However, we insist that a *major objective* of the Socrate team is to *motivate the collaborative research between these axes*, this point is specifically detailed in Section 3.5 . The first one is entitled "Flexible Radio Front-End" and will study new radio front-end research challenges brought up by the arrival of MIMO technologies, and reconfigurable front-ends. The second one, entitled "Multi-user communication", will study how to couple the self-adaptive and distributed signal processing algorithms to cope with the multi-scale dynamics found in cognitive radio systems. The last research axis, entitled "Software Radio Programming Models" is dedicated to embedded software issues related to programming the physical protocols layer on these software radio machines. Figure 3 illustrates the three regions of a transceiver corresponding to the three Socrate axes.

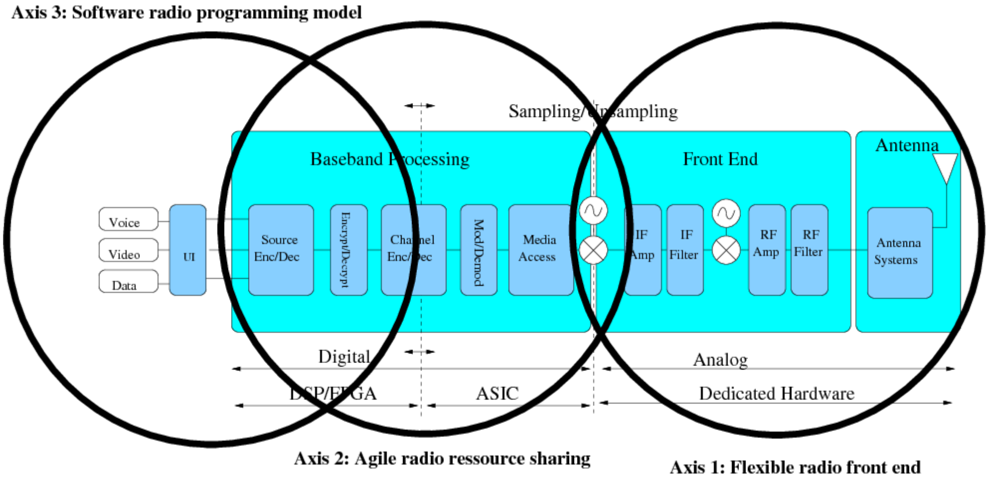


Figure 3. Center of interest for each of the three Socrate research axes with respect to a generic software radio terminal.

3.2. Flexible Radio Front-End

Participants: Guillaume Villemaud, Florin Hutu.

This axis mainly deals with the radio front-end of software radio terminals (right of Fig 3). In order to ensure a high flexibility in a global wireless network, each node is expected to offer as many degrees of freedom as possible. For instance, the choice of the most appropriate communication resource (frequency channel, spreading code, time slot,...), the interface standard or the type of antenna are possible degrees of freedom. The *multi-** paradigm denotes a highly flexible terminal composed of several antennas providing MIMO features to enhance the radio link quality, which is able to deal with several radio standards to offer interoperability and efficient relaying, and can provide multi-channel capability to optimize spectral reuse. On the other hand, increasing degrees of freedom can also increase the global energy consumption, therefore for energy-limited terminals a different approach has to be defined.

In this research axis, we expect to demonstrate optimization of flexible radio front-end by fine grain simulations, and also by the design of home made prototypes. Of course, studying all the components deeply would not be possible given the size of the team, we are currently not working in new technologies for DAC/ADC and power amplifiers which are currently studied by hardware oriented teams. The purpose of this axis is to build system level simulation taking into account the state of the art of each key component.

3.3. Multi-User Communications

Participants: Jean-Marie Gorce, Claire Goursaud, Nikolai Lebedev, Samir Perlaza, Leonardo Sampaio-Cardoso.

While the first and the third research axes deal with the optimization of the cognitive radio nodes themselves from system and programming point of view, an important complementary objective is to consider the radio nodes in their environments. Indeed, cognitive radio does not target the simple optimization of point to point transmissions, but the optimization of simultaneous concurrent transmissions. The tremendous development of new wireless applications and standards currently observed calls for a better management of the radio spectrum with opportunistic radio access, cooperative transmissions and interference management. This challenge has been identified as one of the most important issue for 5G to guarantee a better exploitation of the spectrum. In addition, mobile internet is going to support a new revolution that is the *tactile internet*, with real time interactions between the virtual and the real worlds, requiring new communication objectives to be met such as low latency end to end communications, distributed learning techniques, in-the-network computation, and many more. The future network will be heterogeneous in terms of technologies, type of data flows and QoS requirements. To address this revolution two work directions have naturally formed within the axis. The first direction concerns the theoretical study of fundamental limits in wireless networks. Introduced by Claude Shannon in the 50s and heavily developed up to today, Information Theory has provided a theoretical foundation to study the performance of wireless communications, not from a practical design view point, but using the statistical properties of wireless channels to establish the fundamental trade-offs in wireless communications. Beyond the classical *energy efficiency - spectral efficiency* tradeoff, information theory and its many derivations, i.e., network information theory, may also help to address additional questions such as determining the optimal rates under decentralized policies, asymptotic behavior when the density of nodes increases, latency controled communication with finite block-length theory, etc... In these cases, information theory is often associated to other theoretical tools such as game theory, stochastic geometry, control theory, graph theory and many others.

Our first research direction consists in evaluating specific mulit-user scenarios from a network information theory perspective, inspired by practical scenarios from various applicative frameworks (e.g. 5G, Wifi, sensor networks, IoT, etc...), and to establish fundamental limits for these scenarios. The second research direction is related to algorithmic and protocol design (PHY/MAC), applied to practical scenarios. Exploiting signal processing, linear algebra inspired models and distributed algorithms, we develop and evaluate various distributed algorithms allowing to improve many QoS metrics such as communication rates, reliability, stability, energy efficiency or computational complexity.

It is clear that both research directions are symbiotic with respect to each other, with the former providing theoretical bounds that serves as a reference to the performance of the algorithms created in the later. In the other way around, the later offers target scenarios for the former, through identifying fundamental problems that are interesting to be studied from the fundamental side. Our contributions of the year in these two directions are summarized further in the document.

3.4. Software Radio Programming Model

Participants: Tanguy Risset, Kevin Marquet, Lionel Morel, Guillaume Salagnac, Florent de Dinechin.

Finally the third research axis is concerned with software aspect of the software radio terminal (left of Fig 3). We have currently two actions in this axis, the first one concerns the programming issues in software defined radio devices, the second one focusses on low power devices: how can they be adapted to integrate some reconfigurability.

The expected contributions of Socrate in this research axis are :

- The design and implementation of a “middleware for SDR”, probably based on a Virtual Machine.
- Prototype implementations of novel software radio systems, using chips from Leti and/or Lyrtech software radio boards.
- Development of a *smart node*: a low-power Software-Defined Radio node adapted to WSN applications.
- Methodology clues and programming tools to program all these prototypes.

3.5. Inter-Axes Collaboration

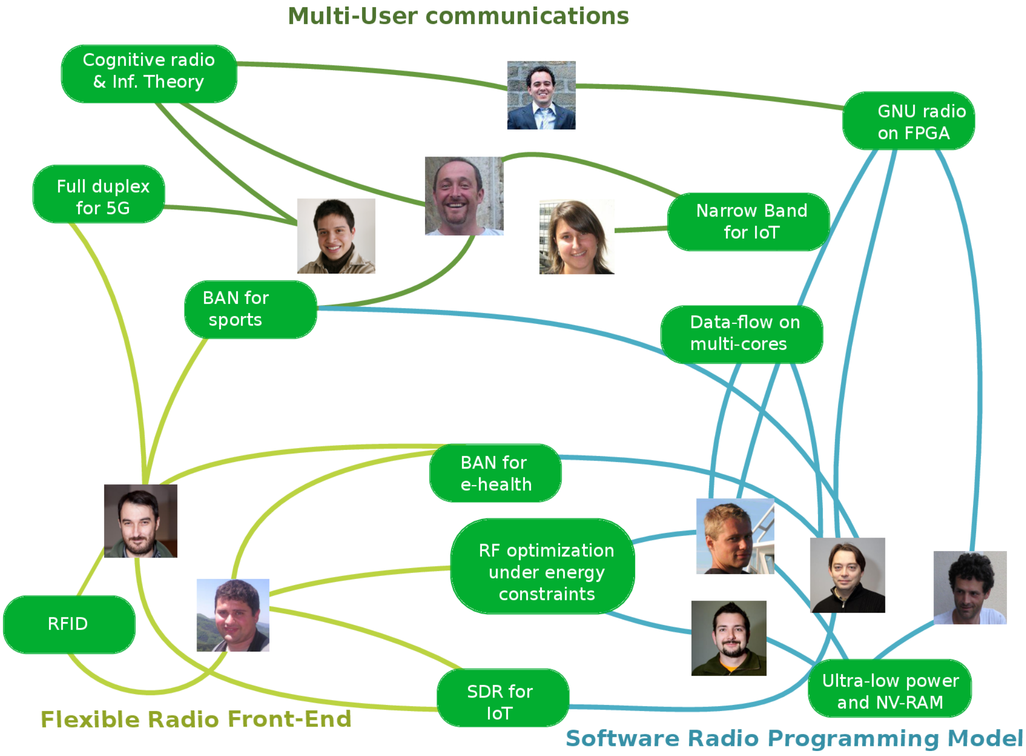

Multi-User communications
Cognitive radio & Inf. Theory
GNU radio on FPGA
Full duplex for 5G
Narrow Band for IoT
BAN for sports
Data-flow on multi-cores
BAN for e-health
RF optimization under energy constraints
RFID
SDR for IoT
Ultra-low power and NV-RAM
Flexible Radio Front-End
Software Radio Programming Model

Figure 4. Inter-Axis Collaboration in Socrate: we expect innovative results to come from this pluri-disciplinary research

Innovative results come from collaborations between the three axes. To highlight the fact that this team structure does not limit the ability of inter-axes collaborations between Socrate members, we list below the *on-going* research actions that *already* involve actors from two or more axes, this is also represented on Fig 4 .

- *Optimizing network capacity of very large scale networks*. 2 Phds started in October/November 2011 with Guillaume Villemaud (axis 1) and Claire Goursaud (axis 2), respectively.
- *SDR for sensor networks*. A PhD started in 2012 in collaboration with FT R&D, involving people from axis 3 (Guillaume Salagnac, Tanguy Risset) and axis 1 (Guillaume Villemaud).
- *CorteXlab*. The 3 axes also collaborate on the design and the development of CorteXlab.

- *body area networks applications*. Axis 2 and axis 3 collaborate on the development of body area networks applications in the framework of the FUI Smacs project. Jean-Marie Gorce and Tanguy Risset co-advised Matthieu Lauzier.
- *Wiplan and NS3*. The MobiSim ADT involves Guillaume Villemaud (axis 1) and Jean-Marie Gorce (axis 2).
- *Resource allocation and architecture of low power multi-band front-end*. The EconHome project involves people from axis 2 (Jean-Marie Gorce,Nikolai Lebedev) and axis 1 (Florin Hutu). 1 Phd started in 2011.
- *Virtual machine for SDR*. In collaboration with CEA, a PhD started in October 2011, involving people from axis 3 (Tanguy Risset, Kevin Marquet) and Leti's engineers closer to axis 2.
- *Relay strategy for cognitive radio*. Guillaume Villemaud and Tanguy Risset were together advisers of Cedric Levy-Bencheton PhD Thesis (defense last June).

Finally, we insist on the fact that the *FIT project* will involve each member of Socrate and will provide many more opportunities to perform cross layer SDR experimentations. FIT is already federating all members of the Socrate team.

3. Research Program

3.1. Introduction

Our research program on self-adaptive software targets two key properties that are detailed in the remainder of this section: *self-healing* and *self-optimization*.

3.2. Objective #1: Self-healing - Mining software artifacts to automatically evolve systems

Software systems are under the pressure of changes all along their lifecycle. Agile development blurs the frontier between design and execution and requires constant adaptation. The size of systems (millions of lines of code) multiplies the number of bugs by the same order of magnitude. More and more systems, such as sensor network devices, live in "surviving" mode, in the sense that they are neither rebootable nor upgradable.

Software bugs are hidden in source code and show up at development-time, testing-time or worse, once deployed in production. Except for very specific application domains where formal proofs are achievable, bugs can not be eradicated. As an order of magnitude, on 16 Dec 2011, the Eclipse bug repository contains 366,922 bug reports. Software engineers and developers work on bug fixing on a daily basis. Not all developers spend the same time on bug fixing. In large companies, this is sometimes a full-time role to manage bugs, often referred to as *Quality Assurance* (QA) software engineers. Also, not all bugs are equal, some bugs are analyzed and fixed within minutes, others may take months to be solved [75].

In terms of research, this means that: (i) one needs means to automatically adapt the design of the software system through automated refactoring and API extraction, (ii) one needs approaches to automate the process of adapting source code in order to fix certain bugs, (iii) one needs to revisit the notion of error-handling so that instead of crashing in presence of errors, software adapts itself to continue with its execution, *e.g.*, in degraded mode.

There is no one-size-fits-all solution for each of these points. However, we think that novel solutions can be found by using **data mining and machine learning techniques tailored for software engineering** [76]. This body of research consists of mining some knowledge about a software system by analyzing the source code, the version control systems, the execution traces, documentation and all kinds of software development and execution artifacts in general. This knowledge is then used within recommendation systems for software development, auditing tools, runtime monitors, frameworks for resilient computing, etc.

The novelty of our approach consists of using and tailoring data mining techniques for analyzing software artifacts (source code, execution traces) in order to achieve the **next level of automated adaptation** (*e.g.*, automated bug fixing). Technically, we plan to mix unsupervised statistical learning techniques (*e.g.* frequent item set mining) and supervised ones (*e.g.* training classifiers such as decision trees). This research is currently not being performed by data mining research teams since it requires a high level of domain expertise in software engineering, while software engineering researchers can use off-the-shelf data mining libraries, such as Weka [61].

We now detail the two directions that we propose to follow to achieve this objective.

3.2.1. Learning from software history how to design software and fix bugs

The first direction is about mining techniques in software repositories (*e.g.*, CVS, SVN, Git). Best practices can be extracted by data mining source code and the version control history of existing software systems. The design and code of expert developers significantly vary from the artifacts of novice developers. We will learn to differentiate those design characteristics by comparing different code bases, and by observing the semantic refactoring actions from version control history. Those design rules can then feed the test-develop-refactor constant adaptation cycle of agile development.

Fault localization of bugs reported in bug repositories. We will build a solid foundation on empirical knowledge about bugs reported in bug repository. We will perform an empirical study on a set of representative bug repositories to identify classes of bugs and patterns of bug data. For this, we will build a tool to browse and annotate bug reports. Browsing will be helped with two kinds of indexing: first, the tool will index all textual artifacts for each bug report; second it will index the semantic information that is not present by default in bug management software—*i.e.*, "contains a stacktrace"). Both indexes will be used to find particular subsets of bug reports, for instance "all bugs mentioning invariants and containing a stacktrace". Note that queries with this kind of complexity and higher are mostly not possible with the state-of-the-art of bug management software. Then, analysts will use annotation features to annotate bug reports. The main outcome of the empirical study will be the identification of classes of bugs that are appropriate for automated localization. Then, we will run machine learning algorithms to identify the latent links between the bug report content and source code features. Those algorithms would use as training data the existing traceability links between bug reports and source code modifications from version control systems. We will start by using decision trees since they produce a model that is explicit and understandable by expert developers. Depending on the results, other machine learning algorithms will be used. The resulting system will be able to locate elements in source code related to a certain bug report with a certain confidence.

Automated bug fix generation with search-based techniques. Once a location in code is identified as being the cause of the bug, we can try to automatically find a potential fix. We envision different techniques: (1) infer fixes from existing contracts and specifications that are violated; (2) infer fixes from the software behavior specified as a test suite; (3) try different fix types one-by-one from a list of identified bug fix patterns; (4) search fixes in a fix space that consists of combinations of atomic bug fixes. Techniques 1 and 2 are explored in [58] and [74]. We will focus on the latter techniques. To identify bug fix patterns and atomic bug fixes, we will perform a large-scale empirical study on software changes (also known as changesets when referring to changes across multiple files). We will develop tools to navigate, query and annotate changesets in a version control system. Then, a grounded theory will be built to master the nature of fixes. Eventually, we will decompose change sets in atomic actions using clustering on changeset actions. We will then use this body of empirical knowledge to feed search-based algorithms (*e.g.* genetic algorithms) that will look for meaningful fixes in a large fix space. To sum up, our research on automated bug fixing will try not only to point to source code locations responsible of a bug, but to search for code patterns and snippets that may constitute the skeleton of a valid patch. Ultimately, a blend of expert heuristics and learned rules will be able to produce valid source code that can be validated by developers and committed to the code base.

3.2.2. Run-time self-healing

The second proposed research direction is about inventing a self-healing capability at run-time. This is complementary to the previous objective that mainly deals with development time issues. We will achieve this in two steps. First, we want to define frameworks for resilient software systems. Those frameworks will help to maintain the execution even in the presence of bugs—*i.e.* to let the system survive. As exposed below, this may mean for example to switch to some degraded modes. Next, we want to go a step further and to define solutions for automated runtime repair, that is, not simply compensating the erroneous behavior, but also determining the correct repair actions and applying them at run-time.

Mining best effort values. A well-known principle of software engineering is the "fail-fast" principle. In a nutshell, it states that as soon as something goes wrong, software should stop the execution before entering incorrect states. This is fine when a human user is in the loop, capable of understanding the error or at least rebooting the system. However, the notion of "failure-oblivious computing" [68] shows that in certain domains, software should run in a resilient mode (*i.e.* capable of recovering from errors) and/or best-effort mode—*i.e.* a slightly imprecise computation is better than stopping. Hence, we plan to investigate data mining techniques in order to learn best-effort values from past executions (*i.e.* somehow learning what is a correct state, or the opposite what is not a completely incorrect state). This knowledge will then be used to adapt the software state and flow in order to mitigate the error consequences, the exact opposite of fail-fast for systems with long-running cycles.

Embedding search based algorithms at runtime. Harman recently described the field of search-based software engineering [62]. We think that certain search based approaches can be embedded at runtime with the goal of automatically finding solutions that avoid crashing. We will create software infrastructures that allow automatically detecting and repairing faults at run-time. The methodology for achieving this task is based on three points: (1) empirical study of runtime faults; (2) learning approaches to characterize runtime faults; (3) learning algorithms to produce valid changes to the software runtime state. An empirical study will be performed to analyze those bug reports that are associated with runtime information (*e.g.* core dumps or stacktraces). After this empirical study, we will create a system that learns on previous repairs how to produce small changes that solve standard runtime bugs (*e.g.* adding an array bound check to throw a handled domain exception rather than a spurious language exception). To achieve this task, component models will be used to (1) encapsulate the monitoring and reparation meta-programs in appropriate components and (2) support runtime code modification using scripting, reflective or bytecode generation techniques.

3.3. Objective #2: Self-optimization - Sharing runtime behaviors to continuously adapt software

Complex distributed systems have to seamlessly adapt to a wide variety of deployment targets. This is due to the fact that developers cannot anticipate all the runtime conditions under which these systems are immersed. A major challenge for these software systems is to develop their capability to continuously reason about themselves and to take appropriate decisions and actions on the optimizations they can apply to improve themselves. This challenge encompasses research contributions in different areas, from environmental monitoring to real-time symptoms diagnosis, to automated decision making. The variety of distributed systems, the number of optimization parameters, and the complexity of decisions often resign the practitioners to design monolithic and static middleware solutions. However, it is now globally acknowledged that the development of dedicated building blocks does not contribute to the adoption of sustainable solutions. This is confirmed by the scale of actual distributed systems, which can—for example—connect several thousands of devices to a set of services hosted in the Cloud. In such a context, the lack of support for smart behaviours at different levels of the systems can inevitably lead to its instability or its unavailability. In June 2012, an outage of Amazon's Elastic Compute Cloud in North Virginia has taken down Netflix, Pinterest, and Instagram services. During hours, all these services failed to satisfy their millions of customers due to the lack of integration of a self-optimization mechanism going beyond the boundaries of Amazon.

The research contributions we envision within this area will therefore be organized as a reference model for engineering **self-optimized distributed systems** autonomously driven by *adaptive feedback control loops*, which will automatically enlarge their scope to cope with the complexity of the decisions to be taken. This solution introduces a multi-scale approach, which first privileges local and fast decisions to ensure the homeostasis [0] property of a single node, and then progressively propagates symptoms in the network in order to reason on a longer term and a larger number of nodes. Ultimately, domain experts and software developers can be automatically involved in the decision process if the system fails to find a satisfying solution. The research program for this objective will therefore focus on the study of mechanisms for **monitoring, taking decisions, and automatically reconfiguring software at runtime and at various scales**. As stated in the self-healing objective, we believe that there is no one-size-fits-all mechanism that can span all the scales of the system. We will therefore study and identify an optimal composition of various adaptation mechanisms in order to produce long-living software systems.

The novelty of this objective is to exploit the wisdom of crowds to define new middleware solutions that are able to continuously adapt software deployed in the wild. We intend to demonstrate the applicability of this approach to distributed systems that are deployed from mobile phones to cloud infrastructures. The key scientific challenges to address can be summarized as follows: *How does software behave once deployed in the wild? Is it possible to automatically infer the quality of experience, as it is perceived by users? Can the*

[0] Homeostasis is the property of a system that regulates its internal environment and tends to maintain a stable, relatively constant condition of properties [Wikipedia].

runtime optimizations be shared across a wide variety of software? How optimizations can be safely operated on large populations of software instances?

The remainder of this section further elaborates on the opportunities that can be considered within the frame of this objective.

3.3.1. Monitoring software in the wild

Once deployed, developers are generally no longer aware of how their software behave. Even if they heavily use testbeds and benchmarks during the development phase, they mostly rely on the bugs explicitly reported by users to monitor the efficiency of their applications. However, it has been shown that contextual artifacts collected at runtime can help to understand performance leaks and optimize the resilience of software systems [77]. Monitoring and understanding the context of software at runtime therefore represent the first building block of this research challenge. Practically, we intend to investigate crowd-sensing approaches, to smartly collect and process runtime metrics (*e.g.*, request throughput, energy consumption, user context). Crowd-sensing can be seen as a specific kind of crowdsourcing activity, which refers to the capability of lifting a (large) diffuse group of participants to delegate the task of retrieving trustable data from the field. In particular, crowd-sensing covers not only *participatory sensing* to involve the user in the sensing task (*e.g.*, surveys), but also *opportunistic sensing* to exploit mobile sensors carried by the user (*e.g.*, smartphones).

While reported metrics generally enclose raw data, the monitoring layer intends to produce meaningful indicators like the *Quality of Experience* (QoE) perceived by users. This QoE reflects representative symptoms of software requiring to trigger appropriate decisions in order to improve its efficiency. To diagnose these symptoms, the system has to process a huge variety of data including runtime metrics, but also history of logs to explore the sources of the reported problems and identify opportunities for optimizations. The techniques we envision at this level encompass machine learning, principal component analysis, and fuzzy logic [67] to provide enriched information to the decision level.

3.3.2. Collaborative decision-making approaches

Beyond the symptoms analysis, decisions should be taken in order to improve the *Quality of Service* (QoS). In our opinion, collaborative approaches represent a promising solution to effectively converge towards the most appropriate optimization to apply for a given symptom. In particular, we believe that exploiting the wisdom of the crowd can help the software to optimize itself by sharing its experience with other software instances exhibiting similar symptoms. The intuition here is that the body of knowledge that supports the optimization process cannot be specific to a single software instance as this would restrain the opportunities for improving the quality and the performance of applications. Rather, we think that any software instance can learn from the experience of others.

With regard to the state-of-the-art, we believe that a multi-levels decision infrastructure, inspired from distributed systems like Spotify [60], can be used to build a decentralized decision-making algorithm involving the surrounding peers before requesting a decision to be taken by more central control entity. In the context of collaborative decision-making, peer-based approaches therefore consist in quickly reaching a consensus on the decision to be adopted by a majority of software instances. Software instances can share their knowledge through a micro-economic model [56], that would weight the recommendations of experienced instances, assuming their age reflects an optimal configuration.

Beyond the peer level, the adoption of algorithms inspired from evolutionary computations, such as genetic programming, at an upper level of decision can offer an opportunity to test and compare several alternative decisions for a given symptom and to observe how does the crowd of applications evolves. By introducing some diversity within this population of applications, some instances will not only provide a satisfying QoS, but will also become naturally resilient to unforeseen situations.

3.3.3. Smart reconfigurations in the large

Any decision taken by the crowd requires to propagate back to and then operated by the software instances. While simplest decisions tend to impact software instances located on a single host (*e.g.*, laptop, smartphone), this process can also exhibit more complex reconfiguration scenarios that require the orchestration of various actions that have to be safely coordinated across a large number of hosts. While it is generally acknowledged that centralized approaches raise scalability issues, we think that self-optimization should investigate different reconfiguration strategies to propagate and apply the appropriate actions. The investigation of such strategies can be addressed in two steps: the consideration of *scalable data propagation protocols* and the identification of *smart reconfiguration mechanisms*.

With regard to the challenge of scalable data propagation protocols, we think that research opportunities encompass not only the exploitation of gossip-based protocols [59], but also the adoption of publish/subscribe abstractions [64] in order to decouple the decision process from the reconfiguration. The fundamental issue here is the definition of a communication substrate that can accommodate the propagation of decisions with relaxed properties, inspired by *Delay Tolerant Networks* (DTN), in order to reach weakly connected software instances. We believe that the adoption of asynchronous communication protocols can provide the sustainable foundations for addressing various execution environments including harsh environments, such as developing countries, which suffer from a partial connectivity to the network. Additionally, we are interested in developing the principle of *social networks of applications* in order to seamlessly group and organize software instances according to their similarities and acquaintances. The underlying idea is that grouping application instances can contribute to the identification of optimization profiles not only contributing to the monitoring layer, but also interested in similar reconfigurations. Social networks of applications can contribute to the anticipation of reconfigurations by exploiting the symptoms of similar applications to improve the performance of others before that problems actually happen.

With regard to the challenge of smart reconfiguration mechanisms, we are interested in building on our established experience of adaptive middleware [72] in order to investigate novel approaches to efficient application reconfigurations. In particular, we are interested in adopting seamless micro-updates and micro-reboot techniques to provide in-situ reconfiguration of pieces of software. Additionally, the provision of safe and secured reconfiguration mechanisms is clearly a key issue that requires to be carefully addressed in order to avoid malicious exploitation of dynamic reconfiguration mechanisms against the software itself. In this area, although some reconfiguration mechanisms integrate transaction models [65], most of them are restricted to local reconfigurations, without providing any support for executing distributed reconfiguration transactions. Additionally, none of the approached published in the literature include security mechanisms to preserve from unauthorized or malicious reconfigurations.

STORM Team

3. Research Program

3.1. Parallel Computing and Architectures

Following the current trends of the evolution of HPC systems architectures, it is expected that future Exascale systems (i.e. Sustaining 10^{18} flops) will have millions of cores. Although the exact architectural details and trade-offs of such systems are still unclear, it is anticipated that an overall concurrency level of $O(10^9)$ threads/tasks will probably be required to feed all computing units while hiding memory latencies. It will obviously be a challenge for many applications to scale to that level, making the underlying system sound like "embarrassingly parallel hardware."

From the programming point of view, it becomes a matter of being able to expose extreme parallelism within applications to feed the underlying computing units. However, this increase in the number of cores also comes with architectural constraints that actual hardware evolution prefigures: computing units will feature extra-wide SIMD and SIMT units that will require aggressive code vectorization or "SIMDization", systems will become hybrid by mixing traditional CPUs and accelerators units, possibly on the same chip as the AMD APU solution, the amount of memory per computing unit is constantly decreasing, new levels of memory will appear, with explicit or implicit consistency management, etc. As a result, upcoming extreme-scale system will not only require unprecedented amount of parallelism to be efficiently exploited, but they will also require that applications generate adaptive parallelism capable to map tasks over heterogeneous computing units.

The current situation is already alarming, since European HPC end-users are forced to invest in a difficult and time-consuming process of tuning and optimizing their applications to reach most of current supercomputers' performance. It will go even worse at horizon 2020 with the emergence of new parallel architectures (tightly integrated accelerators and cores, high vectorization capabilities, etc.) featuring unprecedented degree of parallelism that only too few experts will be able to exploit efficiently. As highlighted by the ETP4HPC initiative, existing programming models and tools won't be able to cope with such a level of heterogeneity, complexity and number of computing units, which may prevent many new application opportunities and new science advances to emerge.

The same conclusion arises from a non-HPC perspective, for single node embedded parallel architectures, combining heterogeneous multicores, such as the ARM big.LITTLE processor and accelerators such as GPUs or DSPs. The need and difficulty to write programs able to run on various parallel heterogeneous architectures has led to initiatives such as HSA, focusing on making it easier to program heterogeneous computing devices. The growing complexity of hardware is a limiting factor to the emergence of new usages relying on new technology.

3.2. Scientific and Societal Stakes

In the HPC context, simulation is already considered as a third pillar of science with experiments and theory. Additional computing power means more scientific results, and the possibility to open new fields of simulation requiring more performance, such as multi-scale, multi-physics simulations. Many scientific domains able to take advantage of Exascale computers, these "Grand Challenges" cover large panels of science, from seismic, climate, molecular dynamics, theoretical and astrophysics physics... Besides, embedded applications are also able to take advantage of these performance increase. There is still an on-going trend where dedicated hardware is progressively replaced by off-the-shelf components, adding more adaptability and lowering the cost of devices. For instance, Error Correcting Codes in cell phones are still hardware chips, but with the forthcoming 5G protocol, new software and adaptative solutions relying on low power multicores are also explored. New usages are also appearing, relying on the fact that large computing capacities are becoming more affordable and widespread. This is the case for instance with Deep Neural Networks where the training phase can be done on supercomputers and then used in embedded mobile systems. The same consideration applies for big data problems, of internet of things, where small sensors provide large amount of data that need to be processed in short amount of time. Even though the computing capacities required for such applications are in general a different scale from HPC infrastructures, there is still a need in the future for high performance computing applications.

However, the outcome of new scientific results and the development of new usages for mobile, embedded systems will be hindered by the complexity and high level of expertise required to tap the performance offered by future parallel heterogeneous architectures.

3.3. Towards More Abstraction

As emphasized by initiatives such as the European Exascale Software Initiative (EESI), the European Technology Platform for High Performance Computing (ETP4HPC), or the International Exascale Software Initiative (IESP), the HPC community needs new programming APIs and languages for expressing heterogeneous massive parallelism in a way that provides an abstraction of the system architecture and promotes high performance and efficiency. The same conclusion holds for mobile, embedded applications that require performance on heterogeneous systems.

This crucial challenge given by the evolution of parallel architectures therefore comes from this need to make high performance accessible to the largest number of developpers, abstracting away architectural details providing some kind of performance portability. Disruptive uses of the new technology and groundbreaking new scientific results will not come from code optimization or task scheduling, but they require the design of new algorithms that require the technology to be tamed in order to reach unprecedented levels of performance.

Runtime systems and numerical libraries are part of the answer, since they may be seen as building blocks optimized by experts and used as-is by application developers. The first purpose of runtime systems is indeed to provide *abstraction*. Runtime systems offer a uniform programming interface for a specific subset of hardware (e.g., OpenGL or DirectX are well-established examples of runtime systems dedicated to hardware-accelerated graphics) or low-level software entities (e.g., POSIX-thread implementations). They are designed as thin user-level software layers that complement the basic, general purpose functions provided by the operating system calls. Applications then target these uniform programming interfaces in a portable manner. Low-level, hardware dependent details are hidden inside runtime systems. The adaptation of runtime systems is commonly handled through drivers. The abstraction provided by runtime systems thus enables portability. Abstraction alone is however not enough to provide portability of performance, as it does nothing to leverage low-level-specific features to get increased performance. Consequently, the second role of runtime systems is to *optimize* abstract application requests by dynamically mapping them onto low-level requests and resources as efficiently as possible. This mapping process makes use of scheduling algorithms and heuristics to decide the best actions to take for a given metric and the application state at a given point in its execution time. This allows applications to readily benefit from available underlying low-level capabilities to their full extent without breaking their portability. Thus, optimization together with abstraction allows runtime systems to offer portability of performance. Numerical libraries provide sets of highly optimized kernels for a given field (dense or sparse linear algebra, FFT, etc.) either in an autonomous fashion or using an underlying runtime system.

Application domains cannot resort to libraries for all codes however, computation patterns such as stencils are a representative example of such difficulty. The compiler technology plays here a central role, in managing high level semantics, either through templates, domain specific languages or annotations. Compiler optimizations, and the same applies for runtime optimizations, are limited by the level of semantics they manage. Providing part of the algorithmic knowledge of an application, for instance knowing that it computes a 5-point stencil and then performs a dot product, would lead to more opportunities to adapt parallelism, memory structures, and is a way to leverage the evolving hardware.

Compilers and runtime play a crucial role in the future of high performance applications, by defining the input language for users, and optimizing/transforming it into high performance code. The objective of STORM is to propose better interactions between compiler and runtime and more semantics for both approaches. We recall in the following section the expertise of the team.

TACOMA Team

3. Research Program

3.1. Collecting pertinent information

In our model, applications adapt their behavior (for instance, the level of automation) to the quality of their perception of the environment. This is important to alleviate the development constraint we usually have on automated system. We "just" have to be sure a given process will always operate at the right automation level given the precision, the completeness or the confidence it has on its own perception. For instance, a car passing through a cross would choose its speed depending on the confidence it has gained during perception data gathering. When it has not enough information or when it could not trust it, it should reduce the automation level, therefore the speed, to only rely on its own sensors. Such adaptation capability shift requirements from the design and deployment (availability, robustness, accuracy, etc.) to the **assessment of the environment perception** we aim to facilitate in this first research axis.

Data characterization. The quality (freshness, accuracy, confidence, reliability, confidentiality, etc.) of the data are of crucial importance to assess the quality of the perception and therefore to ensure proper behavior. The way data is produced, consolidated, and aggregated while flowing to the consumer has an impact on its quality. Moreover part of these quality attributes requires to gather information at several communication layers from various entities. For this purpose, we want to design **lightweight cross-layer interactions** to collect relevant data. As a "frugality" principle should guide our approach, it is not appropriate to build all attributes we can imagine. It is therefore necessary to identify attributes relevant to the application and to have mechanisms to activate/deactivate at run-time the process to collect them.

Data fusion. Raw data should be directly used only to determine low-level abstraction. Further help in abstracting from low-level details can be provided by **data fusion** mechanisms. A good (re)construction of a meaningful information for the application reduces the complexity of the pervasive applications and helps the developers to concentrate on the application logic rather on the management of raw data. Moreover, the reactivity required in pervasive systems and the aggregation of large amounts of data (and its processing) are antagonists. We study **software services that can be deployed closer to the edge of the network**. The exploration of data fusion technics will be guided by different criteria: relevance of abstractions produced for pervasive applications, anonymization of exploited raw data, processing time, etc.

Assessing the correctness of the behavior. To ease the design of new applications and to align the development of new products with the ever faster standard developments, continuous integration could be used in parallel with continuous conformance and interoperability testing. We already participate in the design of new shared platforms that aims at facilitating this providing remote testing tools. Unfortunately, it is not possible to be sure that all potential peers in the surrounding have a conform behavior. Moreover, upon failure or security breach, a piece of equipment could stop to operate properly and lead to global mis-behavior. We want to propose conceptual tools for **testing at runtime devices in the environment**. The result of such conformance or interoperability tests could be stored safely in the environment by authoritative testing entity. Then application could interact with the device with a higher confidence. The confidence level of a device could be part of the quality attribute of the information it contributed to generate. The same set of tools could be used to identify misbehaving device for maintenance purpose or to trigger further testing.

3.2. Building relevant abstraction for new interactions

The pervasive applications are often designed in an ad hoc manner depending on the targeted application area. Ressources (sensors / actuators, connected objets etc.) are often used in silos which complexify the implementation of rich pervasive computing scenarios. In the second research axis, we want to get away from technical aspects identifying **common and reusable system mechanisms** that could be used in various applications.

Tagging the environment. Information relative to environment could be stored by the application itself, but it could be complex to manage for mobile application since it could cross a large number of places with various features. Moreover the developer has to build its own representation of information especially when he wants to share information with other instances of the same application or with other applications. A promising approach is to store and to maintain this information associated to an object or to a place, in the environment itself. The infrastructure should provide services to application developers: add/retrieve information in the environment, share information and control who can access it, add computed properties to object for further usage. We want to study an **extensible model to describe and augment the environment**. Beyond a simple distributed storage, we have in mind a new kind of interaction between pervasive applications and changing environment and between applications themselves.

Taking advantages of the spatial and temporal relationships. To understand the world they have to interact with, pervasive applications often have to (re)built a model of it from the exchange they have with others or from their own observations. A part of the programmer's task consists in building a model of the spatial layout of the objects in the surrounding. The term *layout* can be understood in several ways: the co-location of multiple objects in the same vicinity, the physical arrangement of two objects relative to each other, or even the crossing of an object of a physical area to another, etc. Determining remotely these spatial properties (see figure 1 -a) is difficult without exchanging a lot of information. Properties related to the spatial layout are far easier to characterize locally. They could be abstracted from interaction pattern without any complex virtual representation of the environment (see figure 1 -b). We want to be able to rely on this type of spatial layout in a pervasive environment. In the prior years, the members of TACOMA already worked on **models for processing object interactions** in the physical world to automatically trigger processing. This was the case in particular of the spatial programming principle: physical space is treated as a tuple-space in which objects are automatically synchronized according to their spatial arrangement. We want to follow this approach by considering **richer and more expressive programming models.**

3.3. Acting on the environment

The conceptual tools we aim to study must be *frugal*: they use as less as possible resources, while having the possibility to use much more when it is required. Data needed by an application are not made available for "free"; for example, it costs energy to measure a characteristic of the environment, or to transmit it. So this "design frugality" requires **a fine-grained control** on how data is actually collected from the environment. The third research axis aims at designing solutions that give this control to application developers by **acting on the environment**.

Acting on the data collection. We want to be able to identify which information are reality needed during the perception elaboration process. If a piece of data is missing to build a given information with the appropriate quality level, the data collection mechanism should find relevant information in the environment or modify the way it aggregate it. These could lead to a modification of the behavior of the network layer and the path the piece of data use in the aggregation process.

Acting on object interactions. Object in the environment could adapt their behavior in a way that strongly depend on the object itself and that is difficult to generalize. Beyond the specific behaviors of actuators triggered through specialized or standard interfaces, the production of information required by an application could necessitate an adaptation at the object level (eg. calibration, sampling). The environment should then be able to initiate such adaption transparently to the application, which may not know all objects it passes by.

Adapting object behaviors. The radio communication layers become more flexible and able to adapt the way they use energy to what is really required for a given transmission. We already study how beamforming technics could be used to adapt multicast strategy for video services. We want to show how playing with these new parameters of transmissions (eg. beamforming, power, ...) allows to control spatial relationships objects could have. There is a tradeoff to find between the capacity of the medium, the electromagnetic pollution and the reactivity of the environment. We plan to expend our previous on interface selection and more generally on what we call **opportunistic networking**.

TADAAM Team

3. Research Program

3.1. Need for System-Scale Optimization

Firstly, in order for applications to make the best possible use of the available resources, it is impossible to expose all the low-level details of the hardware to the program, as it would make impossible to achieve portability. Hence, the standard approach is to add intermediate layers (programming models, libraries, compilers, runtime systems, etc.) to the software stack so as to bridge the gap between the application and the hardware. With this approach, optimizing the application requires to express its parallelism (within the imposed programming model), organize the code, schedule and load-balance the computations, etc. In other words, in this approach, the way the code is written and the way it is executed and interpreted by the lower layers drives the optimization. In any case, this approach is centered on how computations are performed. Such an approach is therefore no longer sufficient, as the way an application is executing does depend less and less on the organization of computation and more and more on the way its data is managed.

Secondly, modern large-scale parallel platforms comprise tens to hundreds of thousand nodes [0]. However, very few applications use the whole machine. In general, an application runs only on a subset of the nodes [0]. Therefore, most of the time, an application shares the network, the storage and other resources with other applications running concurrently during its execution. Depending on the allocated resources, it is not uncommon that the execution of one application interferes with the execution of a neighboring one.

Lastly, even if an application is running alone, each element of the software stack often performs its own optimization independently. For instance, when considering an hybrid MPI/OpenMP application, one may realize that threads are concurrently used within the OpenMP runtime system, within the MPI library for communication progression, and possibly within the computation library (BLAS) and even within the application itself (pthreads). However, none of these different classes of threads are aware of the existence of the others. Consequently, the way they are executed, scheduled, prioritized does not depend on their relative roles, their locations in the software stack nor on the state of the application.

The above remarks show that in order to go beyond the state-of-the-art, it is necessary to design a new set of mechanisms allowing cross-layer and system-wide optimizations so as to optimize the way data is allocated, accessed and transferred by the application.

3.2. Scientific Challenges and Research Issues

In TADAAM, we will tackle the problem of efficiently executing an application, at system-scale, on an HPC machine. We assume that the application is already optimized (efficient data layout, use of effective libraries, usage of state-of-the-art compilation techniques, etc.). Nevertheless, even a statically optimized application will not be able to be executed at scale without considering the following dynamic constraints: machine topology, allocated resources, data movement and contention, other running applications, access to storage, etc. Thanks to the proposed layer, we will provide a simple and efficient way for already existing applications, as well as new ones, to express their needs in terms of resource usage, locality and topology, using a high-level semantic.

It is important to note that we target the optimization of each application independently but also several applications at the same time and at system-scale, taking into account their resource requirement, their network usage or their storage access. Furthermore, dealing with code-coupling application is an intermediate use-case that will also be considered.

[0] More than 22,500 XE6 compute node for the BlueWaters system; 5040 B510 Bullx Nodes for the Curie machine; more than 49,000 BGQ nodes for the MIRA machine.

[0] In 2014, the median case was 2048 nodes for the BlueWaters system and, for the first year of the Curie machine, the median case was 256 nodes

Several issues have to be considered. The first one consists in providing relevant **abstractions and models to describe the topology** of the available resources **and the application behavior**.

Therefore, the first question we want to answer is: **“How to build scalable models and efficient abstractions enabling to understand the impact of data movement, topology and locality on performance?”** These models must be sufficiently precise to grasp the reality, tractable enough to enable efficient solutions and algorithms, and simple enough to remain usable by non-hardware experts. We will work on (1) better describing the memory hierarchy, considering new memory technologies; (2) providing an integrated view of the nodes, the network and the storage; (3) exhibiting qualitative knowledge; (4) providing ways to express the multi-scale properties of the machine. Concerning abstractions, we will work on providing general concepts to be integrated at the application or programming model layers. The goal is to offer means, for the application, to express its high-level requirements in terms of data access, locality and communication, by providing abstractions on the notion of hierarchy, mesh, affinity, traffic metrics, etc.

In addition to the abstractions and the aforementioned models we need to **define a clean and expressive API in a scalable way**, in order for applications to express their needs (memory usage, affinity, network, storage access, model refinement, etc.).

Therefore, the second question we need to answer is: “**how to build a system-scale, stateful, shared layer that can gather applications needs expressed with a high-level semantic?**”. This work will require not only to define a clean API where applications will express their needs, but also to define how such a layer will be shared across applications and will scale on future systems. The API will provide a simple yet effective way to express different needs such as: memory usage of a given portion of the code; start of a compute intensive part; phase where the network is accessed intensively; topology-aware affinity management; usage of storage (in read and/or write mode); change of the data layout after mesh refinement, etc. From an engineering point of view, the layer will have a hierarchical design matching the hardware hierarchy, so as to achieve scalability.

Once this has been done, the service layer, will have all the information about the environment characteristics and application requirements. We therefore need to design a set of **mechanisms to optimize applications execution**: communication, mapping, thread scheduling, data partitioning/mapping/movement, etc.

Hence, the last scientific question we will address is: “**How to design fast and efficient algorithms, mechanisms and tools to enable execution of applications at system-scale, in full a HPC ecosystem, taking into account topology and locality?**” A first set of research is related to thread and process placement according to the topology and the affinity. Another large field of study is related to data placement, allocation and partitioning: optimizing the way data is accessed and processed especially for mesh-based applications. The issues of transferring data across the network will also be tackled, thanks to the global knowledge we have on the application behavior and the data layout. Concerning the interaction with other applications, several directions will be tackled. Among these directions we will deal with matching process placement with resource allocation given by the batch scheduler or with the storage management: switching from a best-effort application centric strategy to global optimization scheme.

URBANET Team

3. Research Program

3.1. Capillary networks

The definition of Smart Cities is still constantly redefined and expanded so as to comprehensively describe the future of major urban areas. The Smart City concept mainly refers to granting efficiency and sustainability in densely populated metropolitan areas while enhancing citizens' life and protecting the environment. The Smart City vision can be primarily achieved by a clever integration of ICT in the urban tissue. Indeed, ICTs are enabling an evolution from the current duality between the "real world" and its digitalized counterpart to a continuum in which digital contents and applications are seamlessly interacting with classical infrastructures and services. The general philosophy of smart cities can also be seen as a paradigm shift combining the Internet of Things (IoT) and Machine-to-Machine (M2M) communication with a citizen-centric model, all together leveraging massive data collected by pervasive sensors, connected mobile or fixed devices, and social applications.

The fast expansion of urban digitalization yields new challenges that span from social issues to technical problems. Therefore, there is a significant joint effort by public authorities, academic research communities and industrial companies to understand and address these challenges. Within that context, the application layer, i.e., the novel services that ICT can bring to digital urban environments, have monopolized the attention. Lower-layer network architectures have gone instead quite overlooked. We believe that this might be a fatal error, since the communication network plays a critical role in supporting advanced services and ultimately in making the Smart City vision a reality. The UrbaNet project deals precisely with that aspect, and the study of network solutions for upcoming Smart Cities represents the core of our work.

Most network-related challenges along the road to real-world Smart Cities deal with efficient mobile data communication, both at the backbone and at the radio access levels. It is on the latter that the UrbaNet project is focused. More precisely, the scope of the project maps to that of capillary networks, an original concept we define next.

The capillary networking concept represents a unifying paradigm for wireless last-mile communication in smart cities. The term we use is reminiscent of the pervasive penetration of different technologies for wireless communication in future digital cities. Indeed, capillary networks represent the very last portion of the data distribution and collection network, bringing Internet connectivity to every endpoint of the urban tissue in the same exact way capillary blood vessels bring oxygen and collect carbon dioxide at tissues in the human body. Capillary networks inherit concepts from the self-configuring, autonomous, ad hoc networks so extensively studied in the past decade, but they do so in a holistic way. Specifically, this implies considering multiple technologies and applications at a time, and doing so by accounting for all the specificities of the urban environment.

3.2. Specific issues and new challenges of capillary networks

Capillary networks are not just a collection of independent wireless technologies that can be abstracted from the urban environment and/or studied separately. That approach has been in fact continued over the last decade, as technologies such as sensor, mesh, vehicular, opportunistic, and – generally speaking – M2M networks have been designed and evaluated in isolation and in presence of unrealistic mobility and physical layer, simplistic deployments, random traffic demands, impractical application use cases and non-existent business models. In addition, the physical context of the network has a significant impact on its performances and cannot be reduced to a simple random variable. Moreover, one of the main element of a network never appears in many studies: the user. To summarize, networks issues should be addressed from a user- and context-centric perspective.

Such abstractions and approximations were necessary for understanding the fundamentals of wireless network protocols. However, real world deployments have shown their limits. The finest protocols are often unreliable and hardly applicable to real contexts. That also partially explains the marginal impact of multi-hop wireless technologies on today's production market. Industrial solutions are mostly single-hop, complex to operate, and expensive to maintain.

In the UrbaNet project we consider the capillary network as an ensemble of strongly intertwined wireless networks that are expected to coexist and possibly co-operate in the context of arising digital cities. This has three major implications:

- Each technology contributing to the overall capillary network should not be studied apart. As a matter of fact, mobile devices integrate today a growing number of sensors (e.g., environment sensing, resource consumption metering, movement, health or pollution monitoring) and multiple radio interfaces (e.g., LTE, WiFi, ZigBee,. . .), and this is becoming a trend also in the case of privately owned cars, public transport vehicles, commercial fleets, and even city bikes. Similarly, access network sites tend to implement heterogeneous communication technologies so as to limit capital expenses. Enabling smart-cities needs a dense sensing of its activities, which cannot be achieved without multi-service sensor networks. Moreover, all these devices are expected to inter-operate so as to make the communication more sustainable and reliable. Thus, the technologies that build up the capillary network shall be studied as a whole in the future.
- The capillary network paradigm necessarily accounts for actual urban mobility flows, city land-use layouts, metropolitan deployment constraints, and expected activity of the citizens. Often, these specificities do not arise from purely networking features, but relate to the study of city topologies and road layouts, social acceptability, transportation systems, energy management, or urban economics. Therefore, addressing capillary network scenarios cannot but rely on strong multidisciplinary interactions.
- Digital and smart cities are often characterized by arising M2M applications. However, a city is, before all, the gathering of citizens, who use digital services and mobile Internet for increasing their quality of life, empowerment, and entertainment opportunities. Some data flows should be gathered to, or distributed from, an information system. Some other should be disseminated to a geographically or time constrained perimeter. Future usage may induce peer-to-peer like traffics. Moreover these services are also an enabler of new usages of the urban environment. Solutions built within the capillary network paradigm have to manage this heterogeneity of traffic requirements and user behaviors.

By following these guidelines, the UrbaNet ambition is to go one step beyond traditional approaches discussed above. The capillary network paradigm for Smart Cities is tightly linked to the specificities of the metropolitan context and the citizens' activity. Our proposal is thus to re-think the way capillary network technologies are developed, considering a broader and more practical perspective.

3.3. Characterizing urban networks

Our first objective is to understand and model those properties of real-world urban environments that have an impact on the design, deployment and operation of capillary networks. It means to collect and analyze data from actual deployments and services, as well as testbeds experiments. These data have then to be correlated with urban characteristics, e.g. topography, density of population and activities. The objective is to deduce analytical models, simulations and traces of realistic scenarios that can be leveraged afterward. We structure the axis into three tasks that correspond to the three broad categories of networking aspects affected by the urban context.

- **Topological characteristics**. Nowadays, the way urban wireless network infrastructures are typically represented in the literature is dissatisfying. As an example, wireless links are mostly represented as symmetric, lossless channels whose signal quality depends continuously on the distance between the transmitter and the receiver. No need to say, real-world behaviors are very far from these simplified representations. Another example, topologies are generally modeled according to deterministic (e.g., regular grids and lattices, or perfect hexagonal cell coverages) or stochastic (e.g., random uniform distributions over unbound surfaces) approaches. These make network problems mathematically tractable and simulations easier to set up, but are hardly representative of the layouts encountered in the real world. Employing simplistic models helps understanding some fundamental principles but risks to lead to unreliable results, both from the viewpoint of the network architecture design and from that of its performance evaluation. It is thus our speculation that the actual operations and the real-world topologies of infrastructured capillary networks are key to the successful deployment of these technologies, and, in this task, we aim at characterizing them. To that end, we leverage existing collaborations with device manufacturers (Alcatel-Lucent, HiKob) and operators (Orange), as well as collaboration such as the Sense City project and testbed experiments, in order to provide models that faithfully mimic the behavior of real world network devices. The goal is to understand the important features of the topologies, including, e.g., their overall connectivity level, spatial density, degree distribution, regularity, etc. Building on these results, we try to define network graph models that reproduce such major features and can be employed for the development and evaluation of capillary network solutions.

- **Mobilities**. We aim at understanding and modeling the mobile portion of capillary networks as well as the impact of the human mobility on the network usage. Our definition of “mobile portion” includes traditional mobile users as well as all communication-enabled devices that autonomously interact with Internet-based servers and among themselves. There have been efforts to collect real-world movement traces, to generate synthetic mobility dataset and to derive mobility models. However, real-world traces remain limited to small scenarios or circumstantial subsets of the users (e.g., cabs instead of the whole road traffic). Synthetic traces are instead limited by their scale and by their level of realism, still insufficient. Finally, even the most advanced models cannot but provide a rough representation of user mobility in urban areas, as they do not consider the street layout or the human activity patterns. In the end, although often deprecated, random or stochastic mobility models (e.g., random walks, exponential inter-arrivals and cell residence times) are still the common practice. We are well aware of the paramount importance of a faithful representation of device and user mobility within capillary networks and, in order to achieve it, we leverage a number of realistic sources, including Call Detail Records (CDR) collected by mobile operators, Open Data initiatives, real-world social network data, and experiments. We collect data and analyze it, so as to infer the critical properties of the underlying mobility patterns.
- **Data traffic patterns**. The characterization of capillary network usages means understanding and modeling when, where and how the wireless access provided by the diverse capillary network technologies is exploited by users and devices. In other words, we are interested in learning which applications are used at different geographical locations and day times, which urban phenomena generate network usage, and which kind of data traffic load they induce on the capillary network. Properly characterizing network usages is as critical as correctly modeling network topology and mobility. Indeed, the capillary networks being the link directly collecting the data from end devices, we cannot count on statistical smoothing which yields regular distributions. Unfortunately, the common practice is to consider, e.g., that each user or device generates a constant data traffic or follows on/off models, that the offered load is uniform over space and does not vary over time, that there is small difference between uplink and downlink behaviors, or that source/destination node pairs are randomly distributed in the network. We plan to go further on the specific scenarios we address, such as smart-parking, floating car data, tele-metering, road traffic management of pollution detection. To that end, we collect real-world data, explore it and derive properties useful to the accurate modeling of content consumption.

3.4. Autonomic networking protocols

While the capillary networks concept covers a large panel of technologies, network architectures, applications and services, common challenges remain, regardless the particular choice of a technology or architecture.

Our record of research on spontaneous and multi-hop networks let us think that autonomic networking appears as the main issue: the connectivity to Internet, to cyber-physical systems, to Information Systems should be transparent for the user, context-aware and location-aware. To address these challenges, a capillary network model is required. Unfortunately, very few specific models fit this task today. However, a number of important, specific capillary networks properties can already be inferred from recent experiments: distributed and localized topologies, very high node degree, dynamic network diameter, unstable / asymmetric / non-transitive radio links, concurrent topologies, heterogeneous capabilities, etc. These properties can already be acknowledged in the design of networking solutions, and they are particularly challenging for the functioning of the MAC layer and QoS support. Clearly, capillary networks provide new research opportunities with regard to networking protocols design.

- **Self-* protocols**. In this regard, self-configuration, self-organization and self-healing are some of the major concerns within the context of capillary networks. Solving such issues would allow spontaneous topologies to appear dynamically in order to provide a service depending of the location and the context, while also adapting to the interactions imposed by the urban environment. Moreover, these mechanisms have the capacity to alleviate the management of the network and the deployment engineering rules, and can provide efficient support to the network dynamics due to user mobility, environment modifications, etc. The designed protocols have to be able to react to traffic requests and local node densities. We address such self-adaptive protocols as a transversal solution to several scenarios, e.g. pollution monitoring, smart-services depending on human activities, vehicle to infrastructure communications, etc. In architectures where self-* mechanisms govern the protocol design, both robustness and energy are more than ever essential challenges at the network layer. Solutions such as energy-harvesting can significantly increase the network lifetime in this case, therefore we investigate their impact on the mechanisms at both MAC and network layers.
- **Quality of service issues**. The capillary networks paradigm implies a simultaneous deployment of multiple wireless technologies, and by different entities (industry, local community, citizens). This means that some applications and services can be provided concurrently by different parts of the capillary network, while others might require the cooperation of multiple parties. The notion of Service Level Agreement (SLA) for traffic differentiation, quality of service support (delay, reliability, etc.) is a requirement in these cases for scalability purposes and resource sharing. We contribute to a proper definition of this notion and the related network mechanisms in the settings of low power wireless devices. Because of the urban context, but also because of the wireless media itself, network connectivity is always temporary, while applications require a delivery ratio close to 100%. We investigate different techniques that can achieve this objective in an urban environment.
- **Data impact**. Capillary networks suffer from low capacity facing the increasing user request. In order to cope with network saturation, a promising strategy is to consider the nature of the transmitted data in the development of the protocols. Data aggregation and data gathering are two concepts with a major role to play in this context of limited capacity. In particular, combining local aggregation and measurement redundancy for improving on data reliability is a promising idea, which can also be important for energy saving purposes. Even if the data flow is well known and regular, e.g. temperature or humidity metering, developing aggregation schemes tailored to the constraints of the urban environment is a challenge we address within the UrbaNet team. Many urban applications generate data which has limited spatial and temporal perimeters of relevance, e.g. smart-parking applications, community information broadcasting, etc. When solely a spatial range of relevance is considered, the underlying mechanisms are denoted “geocasting”. We also address these spatio-temporal constraints, which combine geocasting approaches with real-time techniques.

3.5. Optimizing cellular network usage

The capacity of cellular networks, even those that are now being planned, does not seem able to cope with the increasing demands of data users. Moreover, new applications with high bandwidth requirements are also foreseen, for example in the intelligent transportation area, and an exponential growth in signaling traffic is expected in order to enable this data growth. Cumulated with the lack of available new spectrum, this leads to an important challenge for mobile operators, who are looking at both licensed and unlicensed technologies for solutions. The usual strategy consists in a dramatic densification of micro-cells coverage, allowing both to minimize the transmission power of cellular networks as well as to increase the network capacity. However, this solution has obvious physical limits, which we work on determining, and we propose exploiting the capillarity of network interfaces as a complementary solution.

- **Green cellular network**. Increasing the density of micro-cells means multiplying the energy consumption issues. Indeed, the energy consumption of actual LTE eNodeBs and relays, whatever their state, idle, transmitting or receiving, is a major and growing part of the access network energy consumption. For a sustainable deployment of such micro-cell infrastructures and for a significative decrease of the overall energy consumption, an operator needs to be able to switch off cells when they are not absolutely needed. The densification of the cells induces the need for an autonomic control of the on/off state of cells. One solution in this sense can be to adapt the WSN mechanisms to the energy models of micro-cells and to the requirements of a cellular network. The main difficulty here is to be able to adapt and assess the proposed solutions in a realistic environment (in terms of radio propagation, deployment of the cells, user mobility and traffic dynamics).
- **Offloading**. Offloading the cellular infrastructure implies taking advantage of the wealth of connectivity provided by capillary networks instead of relying solely on 4G connectivity. Cellular operators usually possess an important ADSL or cable infrastructure for wired services, the development of femtocell solutions thus becomes very popular. However, while femtocells can be an excellent solution in zones with poor coverage, their extensive use in areas with a high density of mobile users leads to serious interference problems that are yet to be solved. Taking advantage of capillarity for offloading cellular data relies on using IEEE 802.11 Wi-Fi (or other similar technologies) access points or direct device-to-device communications. The ubiquity of Wi-Fi access in urban areas makes this solution particularly interesting, and many studies have focused on its potential. However, these studies fail to take into account the usually low quality of Wi-Fi connections in public areas, and they consider that a certain data rate can be sustained by the Wi-Fi network regardless of the number of contending nodes. In reality, most public Wi-Fi networks are optimized for connectivity, but not for capacity, and more research in this area is needed to correctly assess the potential of this technology. Direct opportunistic communication between mobile users can also be used to offload an important amount of data. This solution raises a number of major problems related to the role of social information and multi-hop communication in the achievable offload capacity. Moreover, in this case the business model is not yet clear, as operators would indeed offload traffic, but also lose revenue as direct ad-hoc communication would be difficult to charge and privacy issues may arise. However, combining hotspot connectivity and multi-hop communications is an appealing answer to broadcasting geo-localized informations efficiently.

WHISPER Project-Team

3. Research Program

3.1. Scientific Foundations

3.1.1. Program analysis

A fundamental goal of the research in the Whisper team is to elicit and exploit the knowledge found in existing code. To do this in a way that scales to a large code base, systematic methods are needed to infer code properties. We may build on either static [33], [36], [39] or dynamic analysis [57], [61], [67]. Static analysis consists of approximating the behavior of the source code from the source code alone, while dynamic analysis draws conclusions from observations of sample executions, typically of test cases. While dynamic analysis can be more accurate, because it has access to information about actual program behavior, obtaining adequate test cases is difficult. This difficulty is compounded for infrastructure software, where many, often obscure, cases must be handled, and external effects such as timing can have a significant impact. Thus, we expect to primarily use static analyses. Static analyses come in a range of flavors, varying in the extent to which the analysis is *sound*, *i.e.*, the extent to which the results are guaranteed to reflect possible run-time behaviors.

One form of sound static analysis is *abstract interpretation* [36]. In abstract interpretation, atomic terms are interpreted as sound abstractions of their values, and operators are interpreted as functions that soundly manipulate these abstract values. The analysis is then performed by interpreting the program in a compositional manner using these abstracted values and operators. Alternatively, *dataflow analysis* [48] iteratively infers connections between variable definitions and uses, in terms of local transition rules that describe how various kinds of program constructs may impact variable values. Schmidt has explored the relationship between abstract interpretation and dataflow analysis [76]. More recently, more general forms of symbolic execution [33] have emerged as a means of understanding complex code. In symbolic execution, concrete values are used when available, and these are complemented by constraints that are inferred from terms for which only partial information is available. Reasoning about these constraints is then used to prune infeasible paths, and obtain more precise results. A number of works apply symbolic execution to operating systems code [29], [31].

While sound approaches are guaranteed to give correct results, they typically do not scale to the very diverse code bases that are prevalent in infrastructure software. An important insight of Engler et al. [41] was that valuable information could be obtained even when sacrificing soundness, and that sacrificing soundness could make it possible to treat software at the scales of the kernels of the Linux or BSD operating systems. Indeed, for certain types of problems, on certain code bases, that may mostly follow certain coding conventions, it may mostly be safe to *e.g.*, ignore the effects of aliases, assume that variable values are unchanged by calls to unanalyzed functions, etc. Real code has to be understood by developers and thus cannot be too complicated, so such simplifying assumptions are likely to hold in practice. Nevertheless, approaches that sacrifice soundness also require the user to manually validate the results. Still, it is likely to be much more efficient for the user to perform a potentially complex manual analysis in a specific case, rather than to implement all possible required analyses and apply them everywhere in the code base. A refinement of unsound analysis is the CEGAR approach [34], in which a highly approximate analysis is complemented by a sound analysis that checks the individual reports of the approximate analysis, and then any errors in reasoning detected by the sound analysis are used to refine the approximate analysis. The CEGAR approach has been applied effectively on device driver code in tools developed at Microsoft [21]. The environment in which the driver executes, however, is still represented by possibly unsound approximations.

Going further in the direction of sacrificing soundness for scalability, the software engineering community has recently explored a number of approaches to code understanding based on techniques developed in the areas of natural language understanding, data mining, and information retrieval. These approaches view code, as well as other software-reated artifacts, such as documentation and postings on mailing lists, as bags of words structured in various ways. Statistical methods are then used to collect words or phrases that seem to be highly correlated, independently of the semantics of the program constructs that connect them. The obliviousness to program semantics can lead to many false positives (invalid conclusions) [53], but can also highlight trends that are not apparent at the low level of individual program statements. We have previously explored combining such statistical methods with more traditional static analysis in identifying faults in the usage of constants in Linux kernel code [52].

3.1.2. Domain Specific Languages

Writing low-level infrastructure code is tedious and difficult, and verifying it is even more so. To produce non-trivial programs, we could benefit from moving up the abstraction stack to enable both programming and proving as quickly as possible. Domain-specific languages (DSLs), also known as *little languages*, are a means to that end [5] [62].

3.1.2.1. Traditional approach.

Using little languages to aid in software development is a tried-and-trusted technique [79] by which programmers can express high-level ideas about the system at hand and avoid writing large quantities of formulaic C boilerplate.

This approach is typified by the Devil language for hardware access [7]. An OS programmer describes the register set of a hardware device in the high-level Devil language, which is then compiled into a library providing C functions to read and write values from the device registers. In doing so, Devil frees the programmer from having to write extensive bit-manipulation macros or inline functions to map between the values the OS code deals with, and the bit-representation used by the hardware: Devil generates code to do this automatically.

However, DSLs are not restricted to being “stub” compilers from declarative specifications. The Bossa language [6] is a prime example of a DSL involving imperative code (syntactically close to C) while offering a high-level of abstraction. This design of Bossa enables the developer to implement new process scheduling policies at a level of abstraction tailored to the application domain.

Conceptually, a DSL both abstracts away low-level details and justifies the abstraction by its semantics. In principle, it reduces development time by allowing the programmer to focus on high-level abstractions. The programmer needs to write less code, in a language with syntax and type checks adapted to the problem at hand, thus reducing the likelihood of errors.

3.1.2.2. Embedding DSLs.

The idea of a DSL has yet to realize its full potential in the OS community. Indeed, with the notable exception of interface definition languages for remote procedure call (RPC) stubs, most OS code is still written in a low-level language, such as C. Where DSL code generators are used in an OS, they tend to be extremely simple in both syntax and semantics. We conjecture that the effort to implement a given DSL usually outweighs its benefit. We identify several serious obstacles to using DSLs to build a modern OS: specifying what the generated code will look like, evolving the DSL over time, debugging generated code, implementing a bug-free code generator, and testing the DSL compiler.

Filet-o-Fish (FoF) [3] addresses these issues by providing a framework in which to build correct code generators from semantic specifications. This framework is presented as a Haskell library, enabling DSL writers to *embed* their languages within Haskell. DSL compilers built using FoF are quick to write, simple, and compact, but encode rigorous semantics for the generated code. They allow formal proofs of the run-time behavior of generated code, and automated testing of the code generator based on randomized inputs, providing greater test coverage than is usually feasible in a DSL. The use of FoF results in DSL compilers that OS developers can quickly implement and evolve, and that generate provably correct code. FoF has been used to build a number of domain-specific languages used in Barrelfish, [22] an OS for heterogeneous multicore systems developed at ETH Zurich.

The development of an embedded DSL requires a few supporting abstractions in the host programming language. FoF was developed in the purely functional language Haskell, thus benefiting from the type class mechanism for overloading, a flexible parser offering convenient syntactic sugar, and purity enabling a more algebraic approach based on small, composable combinators. Object-oriented languages – such as Smalltalk [42] and its descendant Pharo [26] – or multi-paradigm languages – such as the Scala programming language [64] – also offer a wide range of mechanisms enabling the development of embedded DSLs. Perhaps suprisingly, a low-level imperative language – such as C – can also be extended so as to enable the development of embedded compilers [23].

3.1.2.3. Certifying DSLs.

Whilst automated and interactive software verification tools are progressively being applied to larger and larger programs, we have not yet reached the point where large-scale, legacy software – such as the Linux kernel – could formally be proved "correct". DSLs enable a pragmatic approach, by which one could realistically strengthen a large legacy software by first narrowing down its critical component(s) and then focus our verification efforts onto these components.

Dependently-typed languages, such as Coq or Idris, offer an ideal environment for embedding DSLs [32], [27] in a unified framework enabling verification. Dependent types support the type-safe embedding of object languages and Coq's mixfix notation system enables reasonably idiomatic domain-specific concrete syntax. Coq's powerful abstraction facilities provide a flexible framework in which to not only implement and verify a range of domain-specific compilers [3], but also to combine them, and reason about their combination.

Working with many DSLs optimizes the "horizontal" compositionality of systems, and favors reuse of building blocks, by contrast with the "vertical" composition of the traditional compiler pipeline, involving a stack of comparatively large intermediate languages that are harder to reuse the higher one goes. The idea of building compilers from reusable building blocks is a common one, of course. But the interface contracts of such blocks tend to be complex, so combinations are hard to get right. We believe that being able to write and verify formal specifications for the pieces will make it possible to know when components can be combined, and should help in designing good interfaces.

Furthermore, the fact that Coq is also a system for formalizing mathematics enables one to establish a close, formal connection between embedded DSLs and non-trivial domain-specific models. The possibility of developing software in a truly "model-driven" way is an exciting one. Following this methodology, we have implemented a certified compiler from regular expressions to x86 machine code [4]. Interestingly, our development crucially relied on an existing Coq formalization, due to Braibant and Pous, [28] of the theory of Kleene algebras.

While these individual experiments seem to converge toward embedding domain-specific languages in rich type theories, further experimental validation is required. Indeed, Barrelfish is an extremely small software compared to the Linux kernel. The challenge lies in scaling this methodology up to large software systems. Doing so calls for a unified platform enabling the development of a myriad of DSLs, supporting code reuse across DSLs as well as providing support for mechanically-verified proofs.

3.2. Research direction: Tools for improving legacy infrastructure software

A cornerstone of our work on legacy infrastructure software is the Coccinelle program matching and transformation tool for C code. Coccinelle has been in continuous development since 2005. Today, Coccinelle is extensively used in the context of Linux kernel development, as well as in the development of other software, such as wine, python, kvm, and systemd. Currently, Coccinelle is a mature software project, and no research is being conducted on Coccinelle itself. Instead, we leverage Coccinelle in other research projects [24], [25], [65], [68], [72], [74], [78][10], [20], both for code exploration, to better understand at a large scale problems in Linux development, and as an essential component in tools that require program matching and transformation. The continuing development and use of Coccinelle is also a source of visibility in the Linux kernel developer community. We submitted the first patches to the Linux kernel based on Coccinelle in 2007. Since then, over 4500 patches have been accepted into the Linux kernel based on the use of Coccinelle, including around 3000 by over 500 developers from outside our research group.

Our recent work has focused on driver porting. Specifically, we have considered the problem of porting a Linux device driver across versions, particularly backporting, in which a modern driver needs to be used by a client who, typically for reasons of stability, is not able to update their Linux kernel to the most recent version. When multiple drivers need to be backported, they typically need many common changes, suggesting that Coccinelle could be applicable. Using Coccinelle, however, requires writing backporting transformation rules. In order to more fully automate the backporting (or symmetrically forward porting) process, these rules should be generated automatically. We have carried out a preliminary study in this direction with David Lo of Singapore Management University; this work, published at ICSME 2016 [17], is limited to a port from one version to the next one, in the case where the amount of change required is limited to a single line of code. Whisper has been awarded an ANR PRCI grant, to start in March 2017, to collaborate with the group of David Lo on scaling up the rule inference process and proposing a fully automatic porting solution.

3.3. Research direction: developing infrastructure software using Domain Specific Languages

We wish to pursue a *declarative* approach to developing infrastructure software. Indeed, there exists a significant gap between the high-level objectives of these systems and their implementation in low-level, imperative programming languages. To bridge that gap, we propose an approach based on domain-specific languages (DSLs). By abstracting away boilerplate code, DSLs increase the productivity of systems programmers. By providing a more declarative language, DSLs reduce the complexity of code, thus the likelihood of bugs.

Traditionally, systems are built by accretion of several, independent DSLs. For example, one might use Devil [7] to interact with devices, Bossa [6] to implement the scheduling policies. However, much effort is duplicated in implementing the back-ends of the individual DSLs. Our long term goal is to design a unified framework for developing and composing DSLs, following our work on Filet-o-Fish [3]. By providing a single conceptual framework, we hope to amortize the development cost of a myriad of DSLs through a principled approach to reusing and composing them.

Beyond the software engineering aspects, a unified platform brings us closer to the implementation of mechanically-verified DSLs. Dagand's recent work using the Coq proof assistant as an x86 macro-assembler [4] is a step in that direction, which belongs to a larger trend of hosting DSLs in dependent type theories [27], [63], [32]. A key benefit of those approaches is to provide – by construction – a formal, mechanized semantics to the DSLs thus developed. This semantics offers a foundation on which to base further verification efforts, whilst allowing interaction with non-verified code. We advocate a methodology based on incremental, piece-wise verification. Whilst building fully-certified systems from the top-down is a worthwhile endeavor [49], we wish to explore a bottom-up approach by which one focuses first and foremost on crucial subsystems and their associated properties.

Our current work on DSLs has two complementary goals: (i) the design of a unified framework for developing and composing DSLs, following our work on Filet-o-Fish, and (ii) the design of domain-specific languages for domains where there is a critical need for code correctness, and corresponding methodologies for proving properties of the run-time behavior of the system.

ALICE Project-Team

3. Research Program

3.1. Introduction

Computer Graphics is a quickly evolving domain of research. These last few years, both acquisition techniques (*e.g.*, range laser scanners) and computer graphics hardware (the so-called GPU's, for Graphics Processing Units) have made considerable advances. However, despite these advances, fundamental problems still remain open. For instance, a scanned mesh composed of hundred millions triangles cannot be used directly in real-time visualization or complex numerical simulation. To design efficient solutions for these difficult problems, ALICE studies two fundamental issues in Computer Graphics:

- the representation of the objects, *i.e.*, their geometry and physical properties;
- the interaction between these objects and light.

Historically, these two issues have been studied by independent research communities. However, we think that they share a common theoretical basis. For instance, multi-resolution and wavelets were mathematical tools used by both communities [29]. We develop a new approach, which consists in studying the geometry and lighting from the *numerical analysis* point of view. In our approach, geometry processing and light simulation are systematically restated as a (possibly non-linear and/or constrained) functional optimization problem. This type of formulation leads to algorithms that are more efficient. Our long-term research goal is to find a formulation that permits a unified treatment of geometry and illumination over this geometry.

3.2. Geometry Processing for Engineering

Keywords: Mesh processing, parameterization, splines

Geometry processing recently emerged (in the middle of the 90's) as a promising strategy to solve the geometric modeling problems encountered when manipulating meshes composed of hundred millions of elements. Since a mesh may be considered to be a *sampling* of a surface - in other words a *signal* - the *digital signal processing* formalism was a natural theoretic background for this subdomain (see *e.g.*, [30]). Researchers of this domain then studied different aspects of this formalism applied to geometric modeling.

Although many advances have been made in the geometry processing area, important problems still remain open. Even if shape acquisition and filtering is much easier than 30 years ago, a scanned mesh composed of hundred million triangles cannot be used directly in real-time visualization or complex numerical simulation. For this reason, automatic methods to convert those large meshes into higher level representations are necessary. However, these automatic methods do not exist yet. For instance, the pioneer Henri Gouraud often mentions in his talks that the *data acquisition* problem is still open [19]. Malcolm Sabin, another pioneer of the "Computer Aided Geometric Design" and "Subdivision" approaches, mentioned during several conferences of the domain that constructing the optimum control-mesh of a subdivision surface so as to approximate a given surface is still an open problem [28]. More generally, converting a mesh model into a higher level representation, consisting of a set of equations, is a difficult problem for which no satisfying solutions have been proposed. This is one of the long-term goals of international initiatives, such as the AIMShape European network of excellence.

Motivated by gridding application for finite elements modeling for oil and gas exploration, in the frame of the Gocad project, we started studying geometry processing in the late 90's and contributed to this area at the early stages of its development. We developed the LSCM method (Least Squares Conformal Maps) in cooperation with Alias Wavefront [24]. This method has become the de-facto standard in automatic unwrapping, and was adopted by several 3D modeling packages (including Maya and Blender). We explored various applications of the method, including normal mapping, mesh completion and light simulation [21].

However, classical mesh parameterization requires to partition the considered object into a set of topological disks. For this reason, we designed a new method (Periodic Global Parameterization) that generates a continuous set of coordinates over the object [26]. We also showed the applicability of this method, by proposing the first algorithm that converts a scanned mesh into a Spline surface automatically [23].

We are still not fully satisfied with these results, since the method remains quite complicated. We think that a deeper understanding of the underlying theory is likely to lead to both efficient and simple methods. For this reason, in 2012 we studied several ways of discretizing partial differential equations on meshes, including Finite Element Modeling and Discrete Exterior Calculus. In 2013, we also explored Spectral Geometry Processing and Sampling Theory (more on this below).

3.3. Computer Graphics

Keywords: texture synthesis, shape synthesis, texture mapping, visibility

Content creation is one of the major challenges in Computer Graphics. Modeling shapes and surface appearances which are visually appealing and at the same time enforce precise design constraints is a task only accessible to highly skilled and trained designers.

In this context the team focuses on methods for by-example content creation. Given an input example and a set of constraints, we design algorithms that can automatically generate a new shape (geometry+texture). We formulate the problem of content synthesis as the joint optimization of several objectives: Preserving the local appearance of the example, enforcing global objectives (size, symmetries, mechanical properties), reaching user defined constraints (locally specified geometry, contacts). This results in a wide range of optimization problems, from statistical approaches (Markov Random fields), to combinatorial and linear optimization techniques.

As a complement to the design of techniques for automatic content creation, we also work on the representation of the content, so as to allow for its efficient manipulation. In this context we develop data structures and algorithms targeted at massively parallel architectures, such as GPUs. These are critical to reach the interactive rates expected from a content creation technique. We also propose novel ways to store and access content defined along surfaces [27] or inside volumes [18] [22].

The team also continues research in core topics of computer graphics at the heart of realistic rendering and realistic light simulation techniques; for example, mapping textures on surfaces, or devising visibility relationships between 3D objects populating space.

ALPAGE Project-Team

3. Research Program

3.1. From programming languages to linguistic grammars

Participants: Éric Villemonte de La Clergerie, Benoît Sagot, Pierre Boullier, Djamé Seddah, Corentin Ribeyre.

Historically, several members of Alpage were originally specialists in the domain of modeling and parsing for programming languages, and have been working for more than 15 years on the generalization and extension of the techniques involved to the domain of natural language. The shift from programming language grammars to NLP grammars seriously increases complexity (e.g., grammar size [0]) and requires ways to handle the ambiguities inherent in every human language. It is well known that these ambiguities are the sources of many badly handled combinatorial explosions.

Furthermore, while most programming languages are expressed by (subclasses) of well-understood context-free grammars (CFGs), no consensual grammatical formalism has yet been accepted by the whole linguistic community for the description of human languages. On the contrary, new formalisms (or variants of older ones) appear constantly. Many of them may be classified into the three following large families:

Mildly Context-Sensitive (MCS) formalisms They manipulate possibly complex elementary structures with enough restrictions to ensure the possibility of parsing with polynomial time complexities. They include, for instance, Tree Adjoining Grammars (TAGs) and Multi-component TAGs with trees as elementary structures, Linear Indexed Grammars (LIGs). Although they are strictly more powerful than MCS formalisms, Range Concatenation Grammars (RCGs, introduced and used by Alpage members, such as Pierre Boullier and Benoît Sagot [56], [79], [84]) are also parsable in polynomial time.

Unification-based formalisms They combine a context-free backbone with logic arguments as decoration on non-terminals. Most famous representatives are Definite Clause Grammars (DCGs) where PROLOG powerful unification is used to compute and propagate these logic arguments. More recent formalisms, like Lexical Functional Grammars (LFGs) and Head-Driven Phrasal Structure Grammars (HPSGs) rely on more expressive Typed Feature Structures (TFS) or constraints.

Unification-based formalisms with an MCS backbone The two above-mentioned characteristics may be combined, for instance by adding logic arguments or constraints to non-terminals in TAGs.

An efficient way to develop large-coverage hand-crafted symbolic grammars is to use adequate tools and adequate levels of representation, and in particular Meta-Grammars, one of Alpage's areas of expertise, especially with the FRMG grammar and parser for French based on the DyALog logic programming environment [92], [91]. Meta-Grammars (MGs) allows the linguist to focus on a modular description of the linguistic aspects of a grammar, rather than focusing on the specific aspects of a given grammatical formalism. Translation from MGs to grammatical formalisms such as TAG or LFG may be automatically handled. Graphical environments can be used to design MGs and their modularity provides a promising way for sharing the description of common linguistic phenomena across human languages.

3.2. Statistical Parsing

Participants: Djamé Seddah, Marie-Hélène Candito, Benoît Crabbé, Éric Villemonte de La Clergerie, Benoît Sagot, Corentin Ribeyre, Pierre Boullier, Maximin Coavoux.

[0] boullier:2010:inria-00516341:1

Contrary to symbolic approaches to parsing, in statistical parsing, the grammar is extracted from a corpus of syntactic trees : a treebank. The main advantage of the statistical approach is to encode within the same framework the parsing and disambiguating tasks. The extracted grammar rules are associated with probabilities that allow to score and rank the output parse trees of an input sentence. This obvious advantage of probabilistic context-free grammars has long been counterbalanced by two main shortcomings that resulted in poor performance for plain PCFG parsers: (i) the generalization encoded in non terminal symbols that stand for syntagmatic phrases is too coarse (so probabilistic independence between rules is too strong an assertion) and (ii) lexical items are underused. In the last decade though, effective solutions to these shortcomings have been proposed. Symbol annotation, either manual [72] or automatic [75], [76] captures inter-dependence between CFG rules. Lexical information is integrated in frameworks such as head-driven models that allow lexical heads to percolate up the syntagmatic tree [59], or probabilistic models derived from lexicalized Tree Adjoining grammars, such as Stochastic Tree Insertion Grammars [58].

In the same period, totally different parsing architectures have been proposed, to obtain dependency-based syntactic representations. The properties of dependency structures, in which each word is related to exactly one other word, make it possible to define dependency parsing as a sequence of simple actions (such as read buffer and store word on top of a stack, attach read word as dependent of stack top word, attach read word as governor of stack top word ...) [94], [74]. Classifiers can be trained to choose the best action to perform given a partial parsing configuration. In another approach, dependency parsing is cast into the problem of finding the maximum spanning tree within the graph of all possible word-to-word dependencies, and online classification is used to weight the edges [73]. These two kinds of statistical dependency parsing allow to benefit from discriminative learning, and its ability to easily integrate various kinds of features, which is typically needed in a complex task such as parsing.

Statistical parsing is now effective, both for syntagmatic representations and dependency-based syntactic representations. Alpage has obtained state-of-the-art parsing results for French, by adapting various parser learners for French, and works on the current challenges in statistical parsing, namely (1) robustness and portability across domains and (2) the ability to incorporate exogenous data to improve parsing attachment decisions. Alpage is the first French team to have turned the French TreeBank into a resource usable for training statistical parsers, to distribute a dependency version of this treebank, and to make freely available various state-of-the art statistical POS-taggers and parsers for French. We review below the approaches that Alpage has tested and adapted, and the techniques that we plan to investigate to answer these challenges.

In order to investigate statistical parsers for French, we have first worked how to use the French Treebank [53], [52] and derive the best input for syntagmatic statistical parsing [60]. Benchmarking several PCFG-based learning frameworks [86] has led to state-of-the-art results for French, the best performance being obtained with the split-merge Berkeley parser (PCFG with latent annotations) [76].

In parallel to the work on dependency based representation, presented in the next paragraph, we also conducted a preliminary set of experiments on richer parsing models based on Stochastic Tree Insertion Grammars as used in [58] and which, besides their inferior performance compared to PCFG-LA based parser, raise promising results with respect to dependencies that can be extracted from derivation trees. One variation we explored, that uses a specific TIG grammar instance, a *vertical* grammar called *spinal* grammars, exhibits interesting properties wrt the grammar size typically extracted from treebanks (a few hundred unlexicalized trees, compared to 14 000 CFG rules). These models are currently being investigated in our team [89].

Pursuing our work on PCFG-LA based parsing, we investigated the automatic conversion of the treebank into dependency syntax representations [57], that are easier to use for various NLP applications such as question-answering or information extraction, and that are a better ground for further semantic analysis. This conversion can be applied on the treebank, before training a dependency-based parser, or on PCFG-LA parsed trees. This gives the possibility to evaluate and compare on the same gold data, both syntagmatic- and dependency-based statistical parsing. This also paved the way for studies on the influence of various types of lexical information.

3.3. Robust linguistic processing

Participants: Djamé Seddah, Benoît Sagot, Éric Villemonte de La Clergerie, Marie-Hélène Candito, Pierre Magistry.

The constitution of resources such as lexica or grammars raises the issues of the evaluation of these resources to assess their quality and coverage. For this reason, Alpage was the leader of the PASSAGE ANR project (ended in June 2010), which is the follow-up of the EASy parsing evaluation campaign held in 2004 and conducted by team LIR at LIMSI.

However, although developing parsing techniques, grammars (symbolic or probabilistic), and lexica constitute the key efforts towards deep large-scale linguistic processing, these components need to be included inside a full and robust processing chain, able to handle any text from any source, especially out-of-domain text genres. Such texts that exhibit properties (e.g., lexical and syntactic properties) that are different or differently distributed than what is found on standard data (e.g., training corpora for statistical parsers). The development of shallow processing chains, such as SxPipe , is not a trivial task [80]. Obviously, they are often used as such, and not only as pre-processing tools before parsing, since they perform the basic tasks that produce immediately usable results for many applications, such as tokenization, sentence segmentation, spelling correction (e.g., for improving the output of OCR systems), named entity detection, disambiguation and resolution, as well as morphosyntactic tagging.

Still, when used as a preliminary step before parsers, the quality of parsers' results strongly depends on the quality of such chains. This is especially the case, beyond the standard out-of-domain corpora mentioned above, for user-generated content. Indeed, until very recently out-of-domain text genres that have been prioritized have not been Web 2.0 sources, but rather biomedical texts, child language and general fiction (Brown corpus). Adaptation to user-generated content is a particularly difficult instance of the domain adaptation problem since Web 2.0 is not really a domain: it consists of utterances that are often ungrammatical. It even shares some similarities with spoken language [90]. The poor overall quality of texts found on such media lead to weak parsing and even POS-tagging results. This is because user-generated content exhibits both the same issues as other out-of-domain data, but also tremendous issues related to tokenization, typographic and spelling issues that go far beyond what statistical tools can learn from standard corpora. Even lexical specificities are often more challenging than on edited out-of-domain text, as neologisms built using productive morphological derivation, for example, are less frequent, contrarily to slang, abbreviations or technical jargon that are harder to analyse and interpret automatically.

In order to fully prepare a shift toward more robustness, we developed a first version of a richly annotated corpus of user-generated French text, the French Social Media Bank [7], which includes not only POS, constituency and functional information, but also a layer of "normalized" text. This corpus is fully available and constitutes the first data set on Facebook data to date and the first instance of user generated content for a morphologically-rich language. Thanks to the support of the Labex EFL through, we are currently the finalizing the second release of this data set, extending toward a full treebank of over 4,000 sentences.

Besides delivering a new data set, our main purpose here is to be able to compare two different approaches to user-generated content processing: either training statistical models on the original annotated text, and use them on raw new text; or developing normalization tools that help improving the consistency of the annotations, train statistical models on the normalized annotated text, and use them on normalized texts (before un-normalizing them).

However, this raises issues concerning the normalization step. A good sandbox for working on this challenging task is that of POS-tagging. For this purpose, we did leverage Alpage's work on MElt, a state-of-the art POS tagging system [68]. A first round of experiments on English have already led to promising results during the shared task on parsing user-generated content organized by Google in May 2012 [77], as Alpage was ranked second and third [88]. For achieving this result, we brought together a preliminary implementation of a normalization wrapper around the MElt POS tagger followed by a state-of-the art statistical parser improved by several domain adaptation techniques we originally developed for parsing edited out-of-domain texts. Those techniques are based on the unsupervized learning of word clusters *a la* Brown and benefit from morphological treatments (such as lemmatization or desinflection) [87].

One of our objectives is to generalize the use of the normalization wrapper approach to both POS tagging and parsing, for English and French, in order to improve the quality of the output parses. However, this raises several challenges: non-standard contractions and compounds lead to unexpected syntactic structures. A first round of experiments on the French Social Media Bank showed that parsing performance on such data are much lower than expected. This is why, we are actively working to improve on the baselines we established on that matter.

3.4. Dynamic wide coverage lexical resources

Participants: Benoît Sagot, Laurence Danlos, Éric Villemonte de La Clergerie, Marie-Hélène Candito, Lucie Barque, Marianne Djemaa.

Grammatical formalisms and associated parsing generators are useful only when used together with linguistic resources (lexicons, grammars) so as to build operational parsers, especially when considering modern lexically oriented grammatical formalisms. Hence, linguistic resources are the topic of the following section.

However, wide coverage linguistic resources are scarce and expensive, because they are difficult to build, especially when hand-crafted. This observation motivates us to investigate methods, along to manual development techniques, to automatically or semi-automatically acquire, supplement and correct linguistic resources.

Linguistic expertise remains a very important asset to benefit efficiently from such techniques, including those described below. Moreover, linguistically oriented environments with adequate collaborative interfaces are needed to facilitate the edition, comparison, validation and maintenance of large scale linguistic resources. Just to give some idea of the complexity, a syntactic lexicon, as described below, should provide rich information for several tens of thousands of lemma and several hundreds of thousands of forms.

Successful experiments have been conducted by Alpage members with different languages for the automatic acquisition of morphological knowledge from raw corpora [83]. At the syntactic level, work has been achieved on automatic acquisition of atomic syntactic information and automatic detection of errors in the lexicon [95],[6]. At the semantic level, automatic wordnet development tools have been described [78], [93], [71], [69]. All such techniques need of course to be followed by manual validation, so as to ensure high-quality results.

For French, these techniques, and others, have lead some Alpage members to develop one of the main syntactic resources for French, the Le*fff* [81], [85], developed within the Alexina framework. At the semantic level, Alpage members have developed or are developing various syntactico-semantic or semantic resources, including:

- a wordnet for French, the WOLF [82], [70], the first freely available resource of the kind;
- a French FrameNet lexicon (together with an annotated corpus) within the ASFALDA ANR project;
- and a French VerbNet.

In the last few years, Alpage members have shown how to benefit from other more linguistically-oriented resources, such as the Lexique-Grammaire and DICOVALENCE , in order to improve the coverage and quality of the Le*fff* , the WOLF, the French FrameNet lexicon and the French VerbNet. This work is a good example of how Inria and Paris 7 members of Alpage fruitful collaborate: this collaboration between NLP computer scientists and NLP linguists have resulted in significant advances which would have not been possible otherwise.

Moreover, an increasing effort has been made towards multilingual aspects. In particular, Alexina lexicons exist for German, Slovak, Polish, English, Spanish, Persian, Latin (verbs only), Kurmanji Kurdish, Maltese (verbs only, restricted to the so-called first *binyan*) and Khaling, not including freely-available lexicons adapted to the Alexina framework.

3.5. Discourse structures

Participants: Laurence Danlos, Timothée Bernard, Raphaël Salmon.

Until now, the linguistic modeling and automatic processing of sentences has been the main focus of the community. However, many applications would benefit from more large-scale approaches which go beyond the level of sentences. This is not only the case for automatic translation: information extraction/retrieval, summarizing, and other applications do need to resolve anaphora, which in turn can benefit from the availability of hierarchical discourse structures induced by discourse relations (in particular through the notion of right frontier of discourse structures). Moreover, discourse structures are required to extract sequential (chronological, logical,...) or hierarchical representations of events. It is also useful for topic extraction, which in turns can help syntactic and semantic disambiguation.

Although supra-sentential problematics received increasing attention in the last years, there is no satisfying solution to these problems. Among them, anaphora resolution and discourse structures have a far-reaching impact and are domains of expertise of Alpage members. But their formal modeling has now reached a maturity which allows to integrate them, in a near future, inside future Alpage tools, including parsing systems inherited from Atoll.

It is well known that a text is not a random sequence of sentences: sentences are linked the ones to the others by “discourse relations”, which give to the text a hierarchical structure. Traditionally, it is considered that discourse relations are lexicalized by connectors (adverbial connectors like *ensuite*, conjunctions like *parce que*), or are not lexicalized. This vision is however too simple:

- first, some connectors (in particular conjunctions of subordination) introduce pure modifiers and must not be considered as bearing discourse relations,
- second, other elements than connectors can lexicalize discourse relations, in particular verbs like *précéder / to precede* or *causer / to cause*, which have facts or fact eventualities as arguments [62].

There are three main frameworks used to model discourse structures: RST, SDRT, and, more recently, the TAG-based formalism D-LTAG. Inside Alpage, Laurence Danlos has introduced D-STAG (Discourse Synchronous TAGs, [63],[4]), which subsumes in an elegant way both SDRT and RST, to the extent that SDRT and RST structures can be obtained by two different partial projections of D-STAG structures. As done in D-LTAG, D-STAG extends a lexicalized TAG analysis so as to deal with the level of discourse. D-STAG has been fully formalized, and is hence possible to implement (thanks to Synchronous TAG, or even TAG parsers), provided one develops linguistic descriptions in this formalism.

AVIZ Project-Team

3. Research Program

3.1. Scientific Foundations

The scientific foundations of Visual Analytics lie primarily in the domains of Visualization and Data Mining. Indirectly, it inherits from other established domains such as graphic design, Exploratory Data Analysis (EDA), statistics, Artificial Intelligence (AI), Human-Computer Interaction (HCI), and Psychology.

The use of graphic representation to understand abstract data is a goal Visual Analytics shares with Tukey's Exploratory Data Analysis (EDA) [58], graphic designers such as Bertin [46] and Tufte [57], and HCI researchers in the field of Information Visualization [44].

EDA is complementary to classical statistical analysis. Classical statistics starts from a *problem*, gathers *data*, designs a *model* and performs an *analysis* to reach a *conclusion* about whether the data follows the model. While EDA also starts with a problem and data, it is most useful *before* we have a model; rather, we perform visual analysis to discover what kind of model might apply to it. However, statistical validation is not always required with EDA; since often the results of visual analysis are sufficiently clear-cut that statistics are unnecessary.

Visual Analytics relies on a process similar to EDA, but expands its scope to include more sophisticated graphics and areas where considerable automated analysis is required before the visual analysis takes place. This richer data analysis has its roots in the domain of Data Mining, while the advanced graphics and interactive exploration techniques come from the scientific fields of Data Visualization and HCI, as well as the expertise of professions such as cartography and graphic designers who have long worked to create effective methods for graphically conveying information.

The books of the cartographer Bertin and the graphic designer Tufte are full of rules drawn from their experience about how the meaning of data can be best conveyed visually. Their purpose is to find effective visual representation that describe a data set but also (mainly for Bertin) to discover structure in the data by using the right mappings from abstract dimensions in the data to visual ones.

For the last 25 years, the field of Human-Computer Interaction (HCI) has also shown that interacting with visual representations of data in a tight perception-action loop improves the time and level of understanding of data sets. Information Visualization is the branch of HCI that has studied visual representations suitable to understanding and interaction methods suitable to navigating and drilling down on data. The scientific foundations of Information Visualization come from theories about perception, action and interaction.

Several theories of perception are related to information visualization such as the "Gestalt" principles, Gibson's theory of visual perception [51] and Triesman's "preattentive processing" theory [56]. We use them extensively but they only have a limited accuracy for predicting the effectiveness of novel visual representations in interactive settings.

Information Visualization emerged from HCI when researchers realized that interaction greatly enhanced the perception of visual representations.

To be effective, interaction should take place in an interactive loop faster than 100ms. For small data sets, it is not difficult to guarantee that analysis, visualization and interaction steps occur in this time, permitting smooth data analysis and navigation. For larger data sets, more computation should be performed to reduce the data size to a size that may be visualized effectively.

In 2002, we showed that the practical limit of InfoVis was on the order of 1 million items displayed on a screen [49]. Although screen technologies have improved rapidly since then, eventually we will be limited by the physiology of our vision system: about 20 millions receptor cells (rods and cones) on the retina. Another problem will be the limits of human visual attention, as suggested by our 2006 study on change blindness in large and multiple displays [47]. Therefore, visualization alone cannot let us understand very large data sets. Other techniques such as aggregation or sampling must be used to reduce the visual complexity of the data to the scale of human perception.

Abstracting data to reduce its size to what humans can understand is the goal of Data Mining research. It uses data analysis and machine learning techniques. The scientific foundations of these techniques revolve around the idea of finding a good model for the data. Unfortunately, the more sophisticated techniques for finding models are complex, and the algorithms can take a long time to run, making them unsuitable for an interactive environment. Furthermore, some models are too complex for humans to understand; so the results of data mining can be difficult or impossible to understand directly.

Unlike pure Data Mining systems, a Visual Analytics system provides analysis algorithms and processes compatible with human perception and understandable to human cognition. The analysis should provide understandable results quickly, even if they are not ideal. Instead of running to a predefined threshold, algorithms and programs should be designed to allow trading speed for quality and show the tradeoffs interactively. This is not a temporary requirement: it will be with us even when computers are much faster, because good quality algorithms are at least quadratic in time (e.g. hierarchical clustering methods). Visual Analytics systems need different algorithms for different phases of the work that can trade speed for quality in an understandable way.

Designing novel interaction and visualization techniques to explore huge data sets is an important goal and requires solving hard problems, but how can we assess whether or not our techniques and systems provide real improvements? Without this answer, we cannot know if we are heading in the right direction. This is why we have been actively involved in the design of evaluation methods for information visualization [55], [54], [52], [53], [50]. For more complex systems, other methods are required. For these we want to focus on longitudinal evaluation methods while still trying to improve controlled experiments.

3.2. Innovation

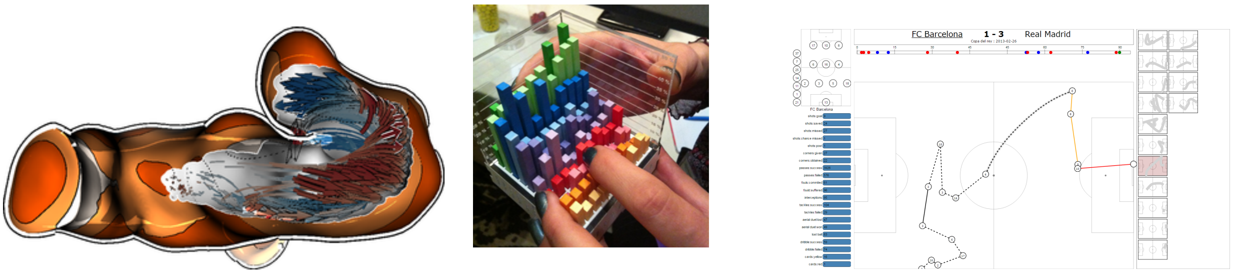


Figure 1. Example novel visualization techniques and tools developed by the team. Left: a non-photorealistic rendering technique that visualizes blood flow and vessel thickness. Middle:a physical visualization showing economic indicators for several countries, right: SoccerStories a tool for visualizing soccer games.

We design novel visualization and interaction techniques (see, for example, Figure 1). Many of these techniques are also evaluated throughout the course of their respective research projects. We cover application domains such as sports analysis, digital humanities, fluid simulations, and biology. A focus of Aviz' work is the improvement of graph visualization and interaction with graphs. We further develop individual techniques for the design of tabular visualizations and different types of data charts. Another focus is the use of animation as a transition aid between different views of the data. We are also interested in applying techniques from illustrative visualization to visual representations and applications in information visualization as well as scientific visualization.

3.3. Evaluation Methods

Evaluation methods are required to assess the effectiveness and usability of visualization and analysis methods. Aviz typically uses traditional HCI evaluation methods, either quantitative (measuring speed and errors) or qualitative (understanding users tasks and activities). Moreover, Aviz is also contributing to the improvement of evaluation methods by reporting on the best practices in the field, by co-organizing workshops (BELIV 2010, 2012, 2014, 2016) to exchange on novel evaluation methods, by improving our ways of reporting, interpreting and communicating statistical results, and by applying novel methodologies, for example to assess visualization literacy.

3.4. Software Infrastructures

We want to understand the requirements that software and hardware architectures should provide to support exploratory analysis of large amounts of data. So far, “big data” has been focusing on issues related to storage management and predictive analysis: applying a well-known set of operations on large amounts of data. Visual Analytics is about exploration of data, with sometimes little knowledge of its structure or properties. Therefore, interactive exploration and analysis is needed to build knowledge and apply appropriate analyses; this knowledge and appropriateness is supported by visualizations. However, applying analytical operations on large data implies long-lasting computations, incompatible with interactions, and generates large amounts of results, impossible to visualize directly without aggregation or sampling. Visual Analytics has started to tackle these problems for specific applications but not in a general manner, leading to fragmentation of results and difficulties to reuse techniques from one application to the other. We are interested in abstracting-out the issues and finding general architectural models, patterns, and frameworks to address the Visual Analytics challenge in more generic ways.

3.5. Emerging Technologies

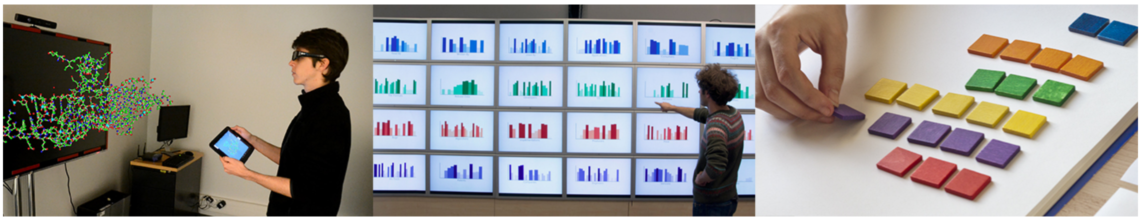


Figure 2. Example emerging technology solutions developed by the team for multi-display environments, wall displays, and token-based visualization.

We want to empower humans to make use of data using different types of display media and to enhance how they can understand and visually and interactively explore information. This includes novel display equipment and accompanying input techniques. The Aviz team specifically focuses on the exploration of the use of large displays in visualization contexts as well as emerging physical and tangible visualizations. In terms of interaction modalities our work focuses on using touch and tangible interaction. Aviz participates to the Digiscope project that funds 11 wall-size displays at multiple places in the Paris area (see http://www.

digiscope.fr), connected by telepresence equipment and a Fablab for creating devices. Aviz is in charge of creating and managing the Fablab, uses it to create physical visualizations, and is also using the local wall-size display (called WILD) to explore visualization on large screens. The team also investigates the perceptual, motor and cognitive implications of using such technologies for visualization.

3.6. Psychology

More cross-fertilization is needed between psychology and information visualization. The only key difference lies in their ultimate objective: understanding the human mind vs. helping to develop better tools. We focus on understanding and using findings from psychology to inform new tools for information visualization. In many cases, our work also extends previous work in psychology. Our approach to the psychology of information visualization is largely holistic and helps bridge gaps between perception, action and cognition in the context of information visualization. Our focus includes the perception of charts in general, perception in large display environments, collaboration, perception of animations, how action can support perception and cognition, and judgment under uncertainty.

AYIN Team

3. Research Program

3.1. Geometric and shape modeling

One of the grand challenges of computer vision and image processing is the expression and use of prior geometric information via the construction of appropriate models. For very high resolution imagery, this problem becomes critically important, as the increasing resolution of the data results in the appearance of a great deal of complex geometric structure hitherto invisible. AYIN studies various approaches to the construction of models of geometry and shape.

3.1.1. Stochastic geometry

One of the most promising approaches to the inclusion of this type of information is stochastic geometry, which is an important research direction in the AYIN team. Instead of defining probabilities for different types of image, probabilities are defined for configurations of an indeterminate number of interacting, parameterized objects located in the image. Such probability distributions are called ‘marked point processes’. New models are being developed both for remote sensing applications, and for skin care problems, such as wrinkle and acne detection.

3.1.2. Contours, phase fields, and MRFs with long-range interactions

An alternative approach to shape modeling starts with generic ‘regions’ in the image, and adds constraints in order to model specific shapes and objects. AYIN investigates contour, phase field, and binary field representations of regions, incorporating shape information via highly-structured long-range interactions that constrain the set of high-probability regions to those with specific geometric properties. This class of models can represent infinite-dimensional families of shapes and families with unbounded topology, as well as families consisting of an arbitrary number of object instances, at no extra computational cost. Key sub-problems include the development of models of more complex shapes and shape configurations; the development of models in more than two spatial dimensions; and understanding the equivalences between models in different representations and approaches.

3.1.3. Shapes in time

AYIN is concerned with spectral and spatio-temporal structures. To deal with the latter, the above scene modeling approaches are extended into the time dimension, either by modeling time dependence directly, or, in the field-based approaches, by modeling spacetime structures, or, in the stochastic geometry approach, by including the time t in the mark. An example is a spatio-temporal graph-cut-based method that introduces directed infinite links connecting pixels in successive image frames in order to impose constraints on shape change.

3.2. Image modeling

The key issue that arises in modeling the high-resolution image data generated in AYIN’s applications, is how to include large-scale spatial, temporal, and spectral dependencies. AYIN investigates approaches to the construction of image models including such dependencies. A central question in the use of such models is how to deal with the large data volumes arising both from the large size of the images involved, and the existence of large image collections. Fortunately, high dimensionality typically implies data redundancy, and so AYIN investigates methods for reducing the dimensionality of the data and describing the spatial, temporal, and spectral dependencies in ways that allow efficient data processing.

3.2.1. Markov random fields with long-range and higher-order interactions

One way to achieve large-scale dependencies is via explicit long-range interactions. MRFs with long-range interactions are also used in AYIN to model geometric spatial and temporal structure, and the techniques and algorithms developed there will also be applied to image modeling. In modeling image structures, however, other important properties, such as control of the relative phase of Fourier components, and spontaneous symmetry breaking, may also be required. These properties can only be achieved by higher-order interactions. These require specific techniques and algorithms, which are developed in parallel with the models.

3.2.2. Hierarchical models

Another way to achieve long-range dependencies is via shorter range interactions in a hierarchical structure. AYIN works on the development of models defined as a set of hierarchical image partitions represented by a binary forest structure. Key sub-problems include the development of multi-feature models of image regions as an ensemble of spectral, texture, geometrical, and classification features, where we search to optimize the ratio between discrimination capacity of the feature space and dimensionality of this space; and the development of similarity criteria between image regions, which would compute distances between regions in the designed feature space and would be data-driven and scale-independent. One way to proceed in the latter case consists in developing a composite kernel method, which would seek to project multi-feature data into a new space, where regions from different thematic categories become linearly or almost linearly separable. This involves developing kernel functions as a combination of basis kernels, and estimating kernel-based support vector machine parameters.

3.3. Algorithms

Computational techniques are necessary in order to extract the information of interest from the models. In addition, most models contain ‘nuisance parameters’, including the structure of the models themselves, that must be dealt with in some way. AYIN is interested in adapting and developing methods for solving these problems in cases where existing methods are inadequate.

3.3.1. Nuisance parameters and parameter estimation

In order to render the models operational, it is crucial to find some way to deal with nuisance parameters. In a Bayesian framework, the parameters must be integrated or marginalized out. Unfortunately, this is usually very difficult. Fortunately, Laplace’s method often provides a good approximation, in many cases being equivalent to classical maximum likelihood parameter estimation. Even these problems are not easy to solve, however, when dealing with complex, structured models. This is particularly true when it is necessary to estimate simultaneously both the information of interest and the parameters. AYIN is developing a number of different methods for dealing with nuisance parameters, corresponding to the diversity of modeling approaches.

3.3.2. Information extraction

Extracting the information of interest from any model involves making estimates based on various criteria, for example MAP, MPM, or MMSE. Computing these estimates often requires the solution of hard optimization problems. The complexity of many of the models to be developed within AYIN means that off-the-shelf algorithms and current techniques are often not capable of solving these problems. AYIN develops a diversity of algorithmic approaches adapted to the particular models developed.

CEDAR Team

3. Research Program

3.1. Scalable Heterogeneous Stores

Big Data applications increasingly involve *diverse* data sources, such as: structured or unstructured documents, data graphs, relational databases etc. and it is often impractical to load (consolidate) diverse data sources in a single repository. Instead, interesting data sources need to be exploited “as they are”, with the added value of the data being realized especially through the ability to combine (join) together data from several sources. Systems capable of exploiting diverse Big Data in this fashion are usually termed *polystores*. A current limitation of polystores is that data stays captive of its original storage system, which may limit the data exploitation performance. We work to devise highly efficient storage systems for heterogeneous data across a variety of data stores.

3.2. Semantic Query Answering

In the presence of data semantics, query evaluation techniques are insufficient as they only take into account the database, but do not provide the reasoning capabilities required in order to reflect the semantic knowledge. In contrast, (ontology-based) query answering takes into account both the data and the semantic knowledge in order to compute the full query answers, blending query evaluation and semantic reasoning.

We aim at designing efficient semantic query answering algorithms, both building on cost-based reformulation algorithms developed in the team and exploring new approaches mixing materialization and reformulation.

3.3. Multi-Model Querying

As the world’s affairs get increasingly more digital, a large and varied set of data sources becomes available: they are either structured databases, such as government-gathered data (demographics, economics, taxes, elections, ...), legal records, stock quotes for specific companies, un-structured or semi-structured, including in particular graph data, sometimes endowed with semantics (see e.g. the Linked Open Data cloud). Modern data management applications, such as data journalism, are eager to combine in innovative ways both static and dynamic information coming from structured, semi-structured, and un-structured databases and social feeds. However, current content management tools for this task are not suited for the task, in particular when they require a lenghy rigid cycle of data integration and consolidation in a warehouse. Thus, we see a need for flexible tools allowing to interconnect various kinds of data sources and to query them together.

3.4. Interactive Data Exploration at Scale

In the Big Data era we are faced with an increasing gap between the fast growth of data and the limited human ability to comprehend data. Consequently, there has been a growing demand of data management tools that can bridge this gap and help users retrieve high-value content from data more effectively. To respond to such user information needs, we aim to build interactive data exploration as a new database service, using an approach called “explore-by-example”.

3.5. Exploratory Querying of Semantic Graphs

Semantic graphs including data and knowledge are hard to apprehend for users, due to the complexity of their structure and oftentimes to their large volumes. To help tame this complexity, in prior research (2014), we have presented a full framework for RDF data warehousing, specifically designed for heterogeneous and semantic-rich graphs. However, this framework still leaves to the users the burden of chosing the most interesting warehousing queries to ask. More user-friendly data management tools are needed, which help the user discover the interesting structure and information hidden within RDF graphs.

3.6. Representative Semantic Query Answering

Top-k search is a classical topic, studied in relational databases, semantic web, recommandation systems,... It is extremely useful, among other, when a human user face a large number of query results, allowing the user to reformulate the query if necessary. However, we argue that top-k search incurs a bias on the perception of the set of results which is out of the control of the user. Our goal is to provide the user with k answers as well which are chosen so as to represent the diversity of the answer set. We will first consider this problem in the setting of relational or RDF databases. We will then extend to more heterogeneous sources, including in particular plain text.

CHROMA Team

3. Research Program

3.1. Introduction

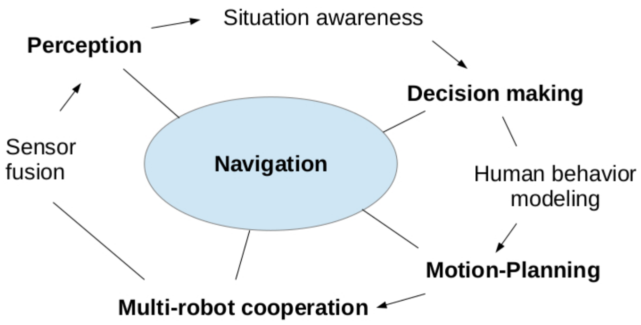


Figure 1. Research themes of the team and their relation

The Chroma team aims to deal with different issues of autonomous mobile robotics : perception, decision-making and cooperation. Figure 1 schemes the different themes and sub-themes investigated by Chroma.

We present here after our approaches to address these different theme of research, and how they combine to contribute to the general problem of robotic navigation. Chroma pays particular attention to current challenges that are autonomous navigation in highly dynamic environments populated by humans and cooperation in (large) multi-robot systems. These challenges are common with other major robotic laboratories/teams in the world, such as Autonomous Systems Lab at ETH Zurich, Robotic Embedded Systems Laboratory at USC, KIT [0] (Prof Christoph Stiller lab and Prof Ruediger Dillmann lab), UC Berkeley, Vislab Parma (Prof. Alberto Broggi), iCeiRA [0] laboratory in Taipei. Chroma is collaborating at various levels (visits, postdocs, research projects, common publications, etc.) with most of these laboratories, see Sections 9.3 and 9.4 .

3.2. Perception and Situation Awareness

Participants: Christian Laugier, Agostino Martinelli, Jilles S. Dibangoye, Anne Spalanzani, Olivier Simonin.

Robust perception in open and dynamic environments populated by human beings is an open and challenging scientific problem. Traditional perception techniques do not provide an adequate solution for these problems, mainly because such environments are uncontrolled [0] and exhibit strong constraints to be satisfied (in particular high dynamicity and uncertainty). This means that **the proposed solutions have to simultaneously take into account characteristics such as real time processing, temporary occultations, dynamic changes or motion predictions**.

[0] Karlsruhe Institut fur Technologie

[0] International Center of Excellence in Intelligent Robotics and Automation Research.

[0] partially unknown and open

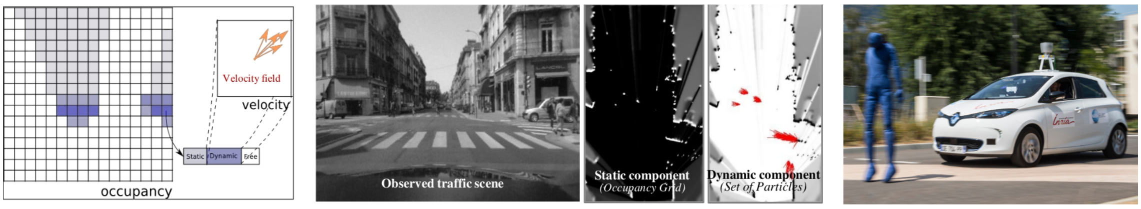


Figure 2. Illustrations of the HSBOF model and experiment with the Zoe car

3.2.1. *Bayesian perception*

Context and previous work. Perception is known to be one of the main bottleneck for robot motion autonomy, in particular when navigating in open and dynamic environments is subject to strong real-time and uncertainty constraints. Traditional object-level solutions [0] still exhibit a lack of efficiency and of robustness when operating in such complex environments. In order to overcome this difficulty, we have proposed in the scope of the former e-Motion team, a new paradigm in robotics called “Bayesian Perception”. The foundation of this approach relies on the concept of “Bayesian Occupancy Filter (BOF)” initially proposed in the PhD thesis of Christophe Coué [42] and further developed in the team [58] [0].

The basic idea is to combine a Bayesian filter with a probabilistic grid representation of both the space and the motions, see illustration Fig. 2 . This new approach can be seen as an extension for uncertain dynamic scenes, of the initial concept of "Occupancy Grid" proposed in 1989 by Elfes [0]. It allows the filtering and the fusion of heterogeneous and uncertain sensors data, by taking into account the history of the sensors measurements, a probabilistic model of the sensors and of the uncertainty, and a dynamic model of the observed objects motions.

In the scope of the Chroma team and of several academic and industrial projects, we went on with the development and the extension under strong embedded implementation constraints, of our Bayesian Perception concept. This work has already led to the development of more powerful models and more efficient implementations, e.g. the *HSBOF*[0] approach [76] and the *CMCDOT*[0] framework [84] which is still under development.

Current and future work address the extension of this model and its software implementation.

Objective — Extending the Bayesian Perception paradigm to the object level — We aim at defining a complete framework extending the Bayesian Perception paradigm to the object level. The main objective is to be simultaneously more robust, more efficient for embedded implementations, and more informative for the subsequent scene interpretation step.

We propose to integrate in a robust way higher level functions such as multiple objects detection and tracking or objects classification. The idea is to avoid well known object level detection errors and data association problems, by simultaneously reasoning at the *grid level* and at the *object level* by extracting / identifying / tracking / classifying clusters of dynamic cells (first work has been published in [84]).

[0] object recognition based on image processing

[0] The *Bayesian programming formalism* developed in e-Motion, pioneered (together with the contemporary work of Thrun, Burgards and Fox [94]) a systematic effort to formalize robotics problems under Probability theory –an approach that is now pervasive in Robotics.

[0] A. Elfes."Occupancy grids: A probabilistic framework for robot perception and navigation", Ph.D. dissertation, Carnegie Mellon University, Pittsburgh, USA, 1989.

[0] Hybrid Sampling Bayesian Occupancy Filter

[0] Conditional Monte Carlo Dense Occupancy Tracker

Software development : new approaches for software / hardware integration The objective is to improve the efficiency of the approach (by exploiting the highly parallel characteristic of our approach), while drastically reducing important factors such as the required memory size, the size of the hardware component, its price and the required energy consumption. This work is absolutely necessary for studying *embedded solutions* for the future generation of mobile robots and autonomous vehicles.

3.2.2. Situation Awareness and Prediction

Context. Prediction of the evolution of the perceived actors is an important ability required for navigation in dynamic and uncertain environments, in particular to allow on-line safe decisions. We have recently shown that an interesting property of the Bayesian Perception approach is to generate short-term conservative [0] predictions on the likely future evolution of the observed scene, even if the sensing information is temporary incomplete or not available [76]. But in human populated environments, estimating more abstract properties (e.g. object classes, affordances, agents intentions) is also crucial to understand the future evolution of the scene.

Objective We aim to develop an integrated approach for "Situation Awareness & Risk Assessment" in complex dynamic scenes involving multiples moving agents (e.g vehicles, cyclists, pedestrians ...), whose behaviors are most of the time unknown but predictable.

Our approach relies on combining machine learning to build a model of the agent behaviors and generic motion prediction techniques (Kalman-based, GHMM [98], Gaussian Processes [92]). A strong challenge of prediction in multiple moving agents environments is to take into consideration the interactions between the different agents (traffic participants). Existing interaction-aware approaches estimate exhaustively the intent of all road users [59], assume a cooperative behavior [88], or learn the policy model of drivers using supervised learning [50]. In contrast, we adopt a *planning-based motion prediction approach*, which is a framework to predict human behavior [102], [56][27]. Planning-based approaches assume that humans, when they perform a task, they do so by minimizing a cost function that depends on their preferences and the context. Such a cost function can be obtained, for example, from demonstrations using *Inverse Reinforcement Learning* [75], [36]. This constitutes an intuitive approach and, more importantly, enables us to overcome the limitations of other approaches, namely, high complexity [59], unrealistic assumptions [88], and overfitting [50]. We have recently demonstrated the predictive potential of our approach in [26].

Towards an On-line Bayesian Decision-Making framework. The team aims at building a general framework for perception and decision-making in multi-robot/vehicle environments. The navigation will be performed under both dynamic and uncertainty constraints, with contextual information and a continuous analysis of the evolution of the probabilistic collision risk (see above). Results have recently been obtained in cooperation with Renault and Berkeley, by using the "Intention / Expectation" paradigm and Dynamic Bayesian Networks; these results have been published in [60], [61] and patented.

We are currently working on the generalization of this approach, in order to take into account the dynamics of the vehicles and multiple traffic participants. The objective is to design a new framework, allowing to overcome the shortcomings of rules-based reasoning approaches usually showing good results [64] [49], but leading to a lack of scalability and long terms predictions. Our research work is carried out through several cooperative projects (Toyota, Renault, project Prefect of IRT Nanoelec, European project ECSEL Enable-S3) and related PhD theses.

3.2.3. Robust state estimation (Sensor fusion)

Context. In order to safely and autonomously navigate in an unknown environment, a mobile robot is required to estimate in real time several physical quantities (e.g., position, orientation, speed). These physical quantities are often included in a common state vector and their simultaneous estimation is usually achieved by fusing the information coming from several sensors (e.g., camera, laser range finder, inertial sensors). The problem of fusing the information coming from different sensors is known as the *Sensor Fusion* problem and it is a fundamental problem which plays a major role in robotics.

[0] i.e. when motion parameters are supposed to be stable during a small amount of time

Objective. A fundamental issue to be investigated in any sensor fusion problem is to understand whether the state is observable or not. Roughly speaking, we need to understand if the information contained in the measurements provided by all the sensors allows us to carry out the estimation of the state. If the state is not observable, we need to detect a new observable state. This is a fundamental step in order to properly define the state to be estimated. To achieve this goal, we apply standard analytic tools developed in control theory together with some new theoretical concepts we introduced in [68] (concept of continuous symmetry). Additionally, we want to account the presence of disturbances in the observability analysis.

Our approach is to introduce general analytic tools able to derive the observability properties in the nonlinear case when some of the system inputs are unknown (and act as disturbances). We recently obtained a simple analytic tool able to account the presence of unknown inputs [71], which extends a heuristic solution derived by the team of Prof. Antonio Bicchi [40] with whom we collaborate (Centro Piaggio at the University of Pisa).

Fusing visual and inertial data. A special attention is devoted to the fusion of inertial and monocular vision sensors (which have strong application for instance in UAV navigation). The problem of fusing visual and inertial data has been extensively investigated in the past. However, most of the proposed methods require a state initialization. Because of the system nonlinearities, lack of precise initialization can irreparably damage the entire estimation process. In literature, this initialization is often guessed or assumed to be known [38], [63], [46]. Recently, this sensor fusion problem has been successfully addressed by enforcing observability constraints [51], [52] and by using optimization-based approaches [62], [45], [66], [53], [74]. These optimization methods outperform filter-based algorithms in terms of accuracy due to their capability of relinearizing past states. On the other hand, the optimization process can be affected by the presence of local minima. We are therefore interested in a deterministic solution that analytically expresses the state in terms of the measurements provided by the sensors during a short time-interval.

For some years we explore deterministic solutions as presented in [69] and [70]. Our objective is to improve the approach by taking into account the biases that affect low-cost inertial sensors (both gyroscopes and accelerometers) and to exploit the power of this solution for real applications. This work is currently supported by the ANR project VIMAD [0] and experimented with a quadrotor UAV. We have a collaboration with Prof. Stergios Roumeliotis (the leader of the MARS lab at the University of Minnesota) and with Prof. Anastasios Mourikis from the University of California Riverside. Regarding the usage of our solution for real applications we have a collaboration with Prof. Davide Scaramuzza (the leader of the Robotics and Perception group at the University of Zurich) and with Prof. Roland Siegwart from the ETHZ.

3.3. Navigation and cooperation in dynamic environments

Participants: Olivier Simonin, Anne Spalanzani, Jilles S. Dibangoye, Christian Laugier, Laetitia Matignon, Fabrice Jumel, Jacques Saraydaryan.

In his reference book *Planning algorithms*[0] S. LaValle discusses the different dimensions that made the motion-planning problem complex, which are the number of robots, the obstacle region, the uncertainty of perception and action, and the allowable velocities. In particular, it is emphasized that complete algorithms require at least exponential time to deal with multiple robot planning in complex environments, preventing them to be scalable in practice (p. 320). Moreover, dynamic and uncertain environments, as human-populated ones, expand this complexity.

In this context, we aim at **scale up decision-making in human-populated environments and in multi-robot systems, while dealing with the intrinsic limits of the robots (computation capacity, limited communication)**.

3.3.1. Motion-planning in human-populated environment

[0] Navigation autonome des drones aériens avec la fusion des données visuelles et inertielles, lead by A. Martinelli, Chroma.

[0] Steven M. LaValle, Planning Algorithms, Cambridge University Press, 2006.

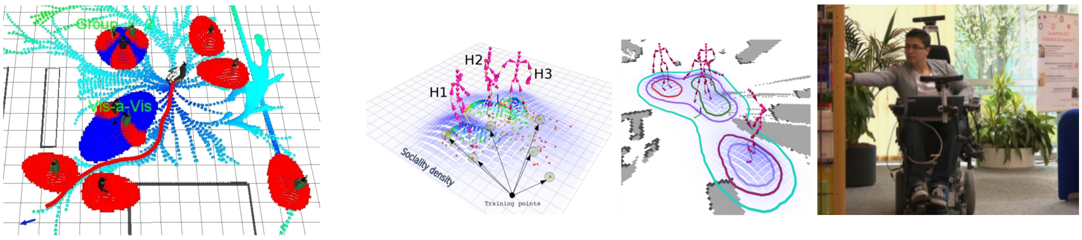


Figure 3. Illustrations of a. the Risk-RRT planning b. the human interaction space model c. experiment with the wheelchair.

Context. Motion planning in dynamic and human-populated environments is a current challenge of robotics. Many research teams work on this topic. We can cite the Institut of robotic in Barcelone [44], the MIT [37], the Autonomous Intelligent Systems lab in Freiburg [41], or the LAAS [77]. In Chroma, we explore different issues : **integrating the risk (uncertainty) in planning processes, modeling and taking into account human behaviors and flows.**

Objective We aim to give the robot some socially compliant behaviors by anticipating the near future (trajectories of mobile obstacle in the robot's surroundings) and by integrating knowledge from psychology, sociology and urban planning. In this context, we will focus on the following 3 topics.

Risk-based planning. Unlike static or controlled environments [0] where global path planning approaches are suitable, dealing with highly dynamic and uncertain environments requires to integrate the notion of risk (risk of collision, risk of disturbance). This risk can be computed by methods proposed in the section 3.2.2 . Then, we examine how motion planning approaches can integrate this risk in the generation and selection of the paths. An algorithm called RiskRRT was proposed in the eMotion team. This algorithm plans goal oriented trajectories that minimize the risk estimated at each instant. It fits environments that are highly dynamic and adapts to a representation of uncertainty [90] (see Figure 3 .a for illustration). Now, we aim to extend this principle to be adapted to various risk evaluation methods (proposed in 3.2) and various situation (highways, urban environments, even in dense traffic or in crowds).

Sharing the physical space with humans. Robots are expected to share their physical space with humans. Hence, robots need to take into account the presence of humans and to behave in a socially acceptable way. Their trajectories must be safe but also predictable, that is why they must follow social conventions, respecting proximity constraints, avoiding people interacting or joining a group engaged in conversation without disturbing. For this purpose, we proposed earlier to integrate some knowledge from the psychology domain (i.e. proxemics theory), see figure 3 .b. We aim now to integrate semantic knowledge [0] and psycho-social theories of human behavior [00] in the navigation framework we have developed for a few years (i.e. the Risk-based navigation algorithms [48], [90], [97]). These concepts were tested on our automated wheelchair (see figure 3 .c) but they have and will be adapted to autonomous cars, telepresence robots and companion robots. This work is currently supported by the ANR Valet, the TENSIVE project and the Associated team Sampen (with Iceira Lab, Taipei).

[0] known environment without uncertainty

[0] B. Kuipers, The Spatial Semantic Hierarchy, Artificial Intelligence, Volume 119, Issues 1–2, May 2000, Pages 191-233

[0] Gibson, J. (1977). The theory of affordances, in Perceiving, Acting, and Knowing. Towards an Ecological Psychology. Number eds Shaw R., Bransford J. Hoboken,NJ: John Wiley & Sons Inc.

[0] Hall, E. (1966). The hidden dimension. Doubleday Anchor Books.

Mapping human flows. We investigate the problem of modeling recurring human displacements to improve robots navigation in such dense populated environments. It has been shown that such recurring behaviours can be mapped from spatial-temporal observations, as in [95]. In this context we address the problem of mapping human flows from robot(s) perception. We started to propose counting-based mapping models [30] that contain motion probabilities in the grid cells. Then such a grid can be exploited to define path-planning functions (eg. A* based) that take into account the probability to encounter humans in opposite direction. We also aim at demonstrating the efficiency of the approach whith real robots evolving in dense human-populated environments.

3.3.2. Decision Making in Multi-robot systems

Context. A central challenge in Chroma is to define **decision-making algorithms that scale up to large multi-robot systems**. This work takes place in the general framework of Multi-Agent Systems (MAS). The objective is to compute/define agent behaviors that provide cooperation and adaptation abilities. Solutions must also take into account the agent/robot computational limits.

We can abstract the challenge in three objectives :
i) mastering the complexity of large fleet of robots/vehicles (scalability),
ii) dealing with limited computational/memory capacity
iii) building adaptive solutions (robustness).

Combining Decision-theoretic models and Swarm intelligence.

Over the past few years, our attempts to address multi-robot decision-making are mainly due to Multi-Agent Sequential Decision Making (MA-SDM) and Swarm Intelligence (SI). MA-SDM builds upon well-known decision-theoretic models (e.g., Markov decision processes and games) and related algorithms, that come with strong theoretical guarantees. In contrast, the expressiveness of MA-SDM models has limited scalability in face of realistic multi-robot systems [0], resulting in computational overload. On their side, SI methods, which rely on local rules – generally bio-inspired – and relating to Self-Organized Systems [0], can scale up to multiple robots and provide robustness to disturbances, but with poor theoretical guarantees [0]. Swarm models can also answer to the need of designing tractable solutions [89], but they remain not geared to express complex realistic tasks or to handle (point-to-point) communication between robots. This motivates our work to go beyond these two approaches and to combine them.

First, we plan to investigate **incremental expansion mechanisms in anytime decision-theoretic planning**, starting from local rules (from SI) to complex strategies with performance guarantees (from MA-SDM) [43]. This methodology is grounded into our research on anytime algorithms, that are guaranteed to stop at anytime while still providing a reliable solution to the original problem. It further relies on decision theoretical models and tools including: Decentralized and Partially Observable Markov Decision Processes and Games, Dynamic Programming, Distributed Reinforcement Learning and Statistical Machine Learning.

Second, we plan to extend the SI approach by considering **the integration of optimization techniques at the local level**. The purpose is to force the system to explore solutions around the current stabilized state – potentially a local optimum – of the system. We aim at keeping scalability and self-organization properties by not compromising the decentralized nature of such systems. Introducing optimization in this way requires to measure locally the performances, which is generally possible from local perception of robots (or using learning techniques). The main optimization methods we will consider are Local Search (Gradient Descent), Distributed Stochastic Algorithm and Reinforcement Learning. We have shown in [96] the interest of such an approach for driverless vehicle traffic optimization. In 2016, we started a new PHD in collaboration with the VOLVO Group to deal with global-local optimization for goods distribution using a fleet of autonomous vehicles.

[0] Martin L. Puterman, Markov Decision Processes; Stuart Russell and Peter Norvig, Artificial Intelligence - A Modern Approach

[0] D. Floreano and C. Mattiussi, Bio-Inspired Artificial Intelligence - Theories, Methods, and Technologies, MIT Press, 2008.

[0] S. A. Brueckner, G. Di Marzo Serugendo, A. Karageorgos, R. Nagpal (2005). Engineering Self-Organising Systems, Methodologies and Applications. LNAI 3464 State-of-the-Art Survey, Springer book.

Both approaches must lead to **master the complexity** inherent to large and open multi-robot systems. Such systems are prone to combinatorial problems, in term of state space and communication, when the number of robots grows. To cope with this complexity we started to develop a methodology which relies on incrementally refining the environment representation while the robots perform their tasks.

Mastering the computational cost involved in cooperative decision-making relies also on building heuristics. We explore how exact (global) solutions can be decentralized in local computation allocated to group of robots or to each robot. We started to apply this methodology to dynamic problems such as the patrolling of moving persons (see [87]).

Beyond this methodological work, we aim to evaluate our models on benchmarks from the literature, by using simulation tools as a complement of robotic experiments. This will lead us to develop simulators, allowing to deploy thousands of humans and robots in constrained environments.

Towards adaptive connected robots.

Mobile robots and autonomous vehicles are becoming more connected to one another and to other devices in the environment (concept of cloud of robots [0] and V2V/V2I connectivity in transportation systems). Such robotic systems are open systems as the number of connected entities is varying dynamically. Network of robots brought with them new problems, as the need of (online) adaption to changes in the system and to the variability of the communication.

In Chroma, we address the problem of adaptation by considering machine learning techniques and local mechanisms as discussed above (SI models). More specifically we investigate the problem of maintaining the connectivity between robots which perform dynamic version of tasks such as patrolling, exploration or transportation, i.e. where the setting of the problem is constinuously changing and growing (see [25]).

Robot fleets should be able to adapt their behavior and organisation to communication limits and variation. It has been shown that wireless communication are very changing in time and space [65]. So we explore how robots can optimize their behaviors by perceiving and learning the quality of their communication in the environment. In Lyon, the CITI Lab. conducts research in many aspects of telecommunication, from signal theory to distributed computation. In this context, Chroma develops cooperations with the Inria team Urbanet [25] (wireless communication protocols) and with the Dynamid team [19] (middlleware and cloud aspects), that we wish to reinforce in the next years.

[0] see for instance the first International Workshop on Cloud and Robotics, 2016.

DAHU Project-Team

3. Research Program

3.1. Research Program

Dahu aims at developing mechanisms for high-level specifications of systems built around DBMS, that are easy to understand while also facilitating verification of critical properties. This requires developing tools that are suitable for reasoning about systems that manipulate data. Some tools for specifying and reasoning about data have already been studied independently by the database community and by the verification community, with various motivations. However, this work is still in its infancy and needs to be further developed and unified.

Most current proposals for reasoning about DBMS over XML documents are based on tree automata, taking advantage of the tree structure of XML documents. For this reason, the Dahu team is studying a variety of tree automata. This ranges from restrictions of "classical" tree automata in order to understand their expressive power, to extensions of tree automata in order to understand how to incorporate the manipulation of data.

Moreover, Dahu is also interested in logical frameworks that explicitly refer to data. Such logical frameworks can be used as high level declarative languages for specifying integrity constraints, format change during data exchange, web service functionalities and so on. Moreover, the same logical frameworks can be used to express the critical properties we wish to verify.

In order to achieve its goals, Dahu brings together world-class expertise in both databases and verification.

DEFROST Team

3. Research Program

3.1. Introduction

Our research crosses different disciplines: numerical mechanics, control design, robotics, optimisation methods, clinical applications. Our organisation aims at facilitating the team work and cross- fertilisation of research results in the group. We have three objectives (1, 2 and 3) that correspond to the main scientific challenges. In addition, we have two transversal objectives that are also highly challenging: the development of a high performance software support for the project (objective 4) and the validation tools and protocols for the models and methods (objective 5).

3.2. Objective 1: Accurate model of soft robot deformation computed in finite time

The objective is to find concrete numerical solutions to the challenge of modelling soft robots with strong real-time constraints. To solve continuum mechanics equations, we will start our research with real-time FEM or equivalent methods that were developed for soft-tissue simulation. We will extend the functionalities to account for the needs of a soft-robotic system:

- Coupling with other physical phenomenons that govern the activity of sensors and actuators (hydraulic, pneumatic, electro-active polymers, shape-memory alloys...).
- Fulfill the new computational time constraints (harder than surgical simulation for training) and find better tradeoff between cost and precision of numerical solvers using reduced-order modelling techniques with error control.
- Exploring interactive and semi-automatic optimisation methods for design based on obtained solution for fast computation on soft robot models.

3.3. Objective 2: Model based control of soft robot behavior

The focus of this objective is on obtaining a generic methodology for soft robot feedback control. Several steps are needed to design a model based control from FEM approach:

- The fundamental question of the kinematic link between actuators, sensors, effectors and contacts us- ing the most reduced mathematical space must be carefully addressed. We need to find efficient algorithms for real-time projection of non-linear FEM models in order to pose the control problem using the only relevant parameters of the motion control.
- Intuitive remote control is obtained when the user directly controls the effector motion. To add this functionality, we need to obtain real-time inverse models of the soft robots by optimisation. Several criteria will be combined in this optimisation: effector motion control, structural stiffness of the robot, reduce intensity of the contact with the environment...
- Investigating closed-loop approaches using sensor feedback: as sensors cannot monitor all points of the deformable structure, the information provided will only be partial. We will need additional algorithms based on the FEM model to obtain the best possible treatment of the information. The final ob- jective of these models and algorithms is to have robust and efficient feedback control strategies for soft robots. One of the main challenge here is to ensure / prove stability in closed-loop.

3.4. Objective 3: Modeling the interaction with a complex environment

Even if the inherent mechanical compliance of soft robots makes them more safe, robust and particularly adapted to interaction with frag- ile environments, the contact forces need to be controlled by:

- Setting up real-time modelling and the control methods needed to pilot the forces that the robot imposes on its environment and to control the robot deformations imposed by its environment. Note that if an operative task requires to apply forces on the surrounding structures, the robot must be anchored to other structures or structurally rigidified.
- Providing mechanics models of the environment that include the uncertainties on the geometry and on the mechanical properties, and are capable of being readjusted in real-time.
- Using the visual feedback of the robot behavior to adapt dynamically the models. The observation provided in the image coupled with an inverse accurate model of the robot could transform the soft robot into sensor: as the robot deforms with the contact of the surroundings, we could retrieve some missing parameters of the environment by a smart monitoring of the robot deformations.

3.5. Objective 4: Soft Robotic Software

Expected research results of this project are numerical methods and algorithms that require high-performance computing and suitability with robotic applications. There is no existing software support for such development. We propose to develop our own software, in a suite split into three applications:

- The first one will facilitate the design of deformable robots by an easy passage from CAD software (for the design of the robot) to the FEM based simulation
- The second one is an anticipative clinical simulator. The aim is to co-design the robotic assistance with the physicians, thanks to a realistic simulation of the procedure or the robotic assistance. This will facilitate the work of reflection on new clinical approaches prior any manufacturing
- The third one is the control design software. It will provide the real-time solutions for soft robot control developed in the project.

3.6. Objective 5: Validation and application demonstrations

The implementation of experimental valida- tion is a key challenge for the project. On one side, we need to validate the model and control algorithms using concrete test case example in order to improve the modelling and to demonstrate the concrete feasibility of our methods. On the other side, concrete applications will also feed the reflexions on the objec- tives of the scientific program.

We will build our own experimental soft robots for the validation of objective 2 and 3 when there is no existing « turn-key » solution. Designing and making our own soft robots, even if only for validation, will help the setting-up of adequate models.

For the validation of objective 4, we will develop « anatomical soft robot »: soft robot with the shape of organs, equipped with sensors (to measure the contact forces) and actuators (to be able to stiffen the walls and recreate natural motion of soft-tissues). We will progressively increase the level of realism of this novel validation set-up to come closer to the anatomical properties.

EX-SITU Team

3. Research Program

3.1. Research Program

We characterize Extreme Situated Interaction as follows:

Extreme users. We study extreme users who make extreme demands on current technology. We know that human beings take advantage of the laws of physics to find creative new uses for physical objects. However, this level of adaptability is severely limited when manipulating digital objects. Even so, we find that creative professionals—artistists, designers and scientists—often adapt interactive technology in novel and unexpected ways and find creative solutions. By studying these users, we hope to not only address the specific problems they face, but also to identify the underlying principles that will help us to reinvent virtual tools. We seek to shift the paradigm of interactive software, to establish the laws of interaction that significantly empower users and allow them to control their digital environment.

Extreme situations. We develop extreme environments that push the limits of today's technology. We take as given that future developments will solve “practical" problems such as cost, reliability and performance and concentrate our efforts on interaction in and with such environments. This has been a successful strategy in the past: Personal computers only became prevalent after the invention of the desktop graphical user interface. Smartphones and tablets only became commercially successful after Apple cracked the problem of a usable touch-based interface for the iPhone and the iPad. Although wearable technologies, such as watches and glasses, are finally beginning to take off, we do not believe that they will create the major disruptions already caused by personal computers, smartphones and tablets. Instead, we believe that future disruptive technologies will include fully interactive paper and large interactive displays.

Our extensive experience with the Digiscope WILD and WILDER platforms places us in a unique position to understand the principles of distributed interaction that extreme environments call for. We expect to integrate, at a fundamental level, the collaborative capabilities that such environments afford. Indeed almost all of our activities in both the digital and the physical world take place within a complex web of human relationships. Current systems only support, at best, passive sharing of information, e.g., through the distribution of independent copies. Our goal is to support active collaboration, in which multiple users are actively engaged in the lifecycle of digital artifacts.

Extreme design. We explore novel approaches to the design of interactive systems, with particular emphasis on extreme users in extreme environments. Our goal is to empower creative professionals, allowing them to act as both designers and developers throughout the design process. Extreme design affects every stage, from requirements definition, to early prototyping and design exploration, to implementation, to adaptation and appropriation by end users. We hope to push the limits of participatory design to actively support creativity at all stages of the design lifecycle.

Extreme design does not stop with purely digital artifacts. The advent of digital fabrication tools and FabLabs has significantly lowered the cost of making physical objects interactive. Creative professionals now create hybrid interactive objects that can be tuned to the user's needs. Integrating the design of physical objects into the software design process raises new challenges, with new methods and skills to support this form of extreme prototyping.

Our overall approach is to identify a small number of specific projects, organized around four themes: *Creativity, Augmentation, Collaboration* and *Infrastructure*. Specific projects may address multiple themes, and different members of the group work together to advance these different topics.

EXMO Project-Team

3. Research Program

3.1. Knowledge representation semantics

We work with semantically defined knowledge representation languages (like description logics, conceptual graphs and object-based languages). Their semantics is usually defined within model theory initially developed for logics. The languages dedicated to the semantic web (RDF and OWL) follow that approach. RDF is a knowledge representation language dedicated to the description of resources; OWL is designed for expressing ontologies: it describes concepts and relations that can be used within RDF.

We consider a language L as a set of syntactically defined expressions (often inductively defined by applying constructors over other expressions). A representation ($o \subseteq L$) is a set of such expressions. It is also called an ontology. An interpretation function (I) is inductively defined over the structure of the language to a structure called interpretation domain (D). This expresses the construction of the "meaning" of an expression in function of its components. A formula is satisfied by an interpretation if it fulfills a condition (in general being interpreted over a particular subset of the domain). A model of a set of expressions is an interpretation satisfying all these expressions. An expression (δ) is then a consequence of a set of expressions (o) if it is satisfied by all of their models (noted $o \models \delta$).

A computer must determine if a particular expression (taken as a query, for instance) is the consequence of a set of axioms (a knowledge base). For that purpose, it uses programs, called provers, that can be based on the processing of a set of inference rules, on the construction of models or on procedural programming. These programs are able to deduce theorems (noted $o \vdash \delta$). They are said to be sound if they only find theorems which are indeed consequences and to be complete if they find all the consequences as theorems. However, depending on the language and its semantics, the decidability, i.e., the ability to create sound and complete provers, is not warranted. Even for decidable languages, the algorithmic complexity of provers may prohibit their exploitation.

To solve this problem a trade-off between the expressivity of the language and the complexity of its provers has to be found. These considerations have led to the definition of languages with limited complexity – like conceptual graphs and object-based representations – or of modular families of languages with associated modular prover algorithms – like description logics.

EXMO mainly considers languages with well-defined semantics (such as RDF and OWL that we contributed to define), and defines the semantics of some languages such as the SPARQL query language and alignment languages, in order to establish the properties of computer manipulations of the representations.

3.2. Ontology matching and alignments

When different representations are used, it is necessary to identify their correspondences. This task is called ontology matching and its result is an alignment [4]. It can be described as follows: given two ontologies, each describing a set of discrete entities (which can be classes, properties, rules, predicates, etc.), find the relationships, if any, holding between these entities.

An alignment between two ontologies o and o' is a set of correspondences $\langle e, e', r\rangle$ such that:

- e and e' are the entities between which a relation is asserted by the correspondence, e.g., formulas, terms, classes, individuals;
- r is the relation asserted to hold between e and e'. This relation can be any relation applying to these entities, e.g., equivalence, subsumption.

In addition, a correspondence may support various types of metadata, in particular measures of the confidence in a correspondence.

Given the semantics of the two ontologies provided by their consequence relation, we define an interpretation of two aligned ontologies as a pair of interpretations $\langle m, m' \rangle$, one for each ontology. Such a pair of interpretations is a model of the aligned ontologies o and o' if and only if each respective interpretation is a model of the ontology and they satisfy all correspondences of the alignment.

This definition is extended to networks of ontologies: a collection of ontologies and associated alignments. A model of such an ontology network is a tuple of local models such that each alignment is valid for the models involved in the tuple. In such a system, alignments play the role of model filters which select the local models that are compatible with all alignments. So, given an ontology network, it is possible to interpret it.

However, given a set of ontologies, it is necessary to find the alignments between them and the semantics does not tell which ones they are. Ontology matching aims at finding these alignments. A variety of methods is used for this task. They perform pairwise comparisons of entities from each of the ontologies and select the most similar pairs. Most matching algorithms provide correspondences between named entities, more rarely between compound terms. The relationships are generally equivalence between these entities. Some systems are able to provide subsumption relations as well as other relations in the support language (like incompatibility or instantiation). Confidence measures are usually given a value between 0 and 1 and are used for expressing preferences between two correspondences.

3.3. Data interlinking

Links are important for the publication of RDF data on the web. We call data interlinking the process of generating links identifying the same resource described in two data sets. Data interlinking parallels ontology matching: from two datasets (d and d') it generates a set of links (also called a link set, L).

We have extended the notion of database keys in a way which is more adapted to the context of description logics and the openness of the semantic web. We have introduced the notion of a link key [4], [1] which is a combination of such keys with alignments. More precisely, a link key is a structure $\langle K^{eq}, K^{in}, C \rangle$ such that:

- K^{eq} is a set of pairs of property expressions;
- K^{in} is a set of pairs of property expressions;
- C is a correspondence between classes.

Such a link key holds if and only if for any pair of resources belonging to the classes in correspondence such that the values of their property in K^{eq} are pairwise equal and the values of those in K^{in} pairwise intersect, the resources are the same.

As can be seen, link key validity is only relying on pairs of objects in two different data sets. We further qualify link keys as weak, plain and strong depending on them satisfying further constraints: a weak link key is only valid on pairs of individuals of different data sets, a plain link key has to apply in addition to pairs of individuals of the same data set as soon as one of them is identified with another individual of the other data set, a strong link key is a link key which is also a key for each data set, it can be though of as a link key which is made of two keys.

Link keys can then be used for finding equal individuals across two data sets and generating the corresponding owl:sameAs links.

FLOWERS Project-Team

3. Research Program

3.1. Research Program

Research in artificial intelligence, machine learning and pattern recognition has produced a tremendous amount of results and concepts in the last decades. A blooming number of learning paradigms - supervised, unsupervised, reinforcement, active, associative, symbolic, connectionist, situated, hybrid, distributed learning... - nourished the elaboration of highly sophisticated algorithms for tasks such as visual object recognition, speech recognition, robot walking, grasping or navigation, the prediction of stock prices, the evaluation of risk for insurances, adaptive data routing on the internet, etc... Yet, we are still very far from being able to build machines capable of adapting to the physical and social environment with the flexibility, robustness, and versatility of a one-year-old human child.

Indeed, one striking characteristic of human children is the nearly open-ended diversity of the skills they learn. They not only can improve existing skills, but also continuously learn new ones. If evolution certainly provided them with specific pre-wiring for certain activities such as feeding or visual object tracking, evidence shows that there are also numerous skills that they learn smoothly but could not be "anticipated" by biological evolution, for example learning to drive a tricycle, using an electronic piano toy or using a video game joystick. On the contrary, existing learning machines, and robots in particular, are typically only able to learn a single pre-specified task or a single kind of skill. Once this task is learnt, for example walking with two legs, learning is over. If one wants the robot to learn a second task, for example grasping objects in its visual field, then an engineer needs to re-program manually its learning structures: traditional approaches to task-specific machine/robot learning typically include engineer choices of the relevant sensorimotor channels, specific design of the reward function, choices about when learning begins and ends, and what learning algorithms and associated parameters shall be optimized.

As can be seen, this requires a lot of important choices from the engineer, and one could hardly use the term "autonomous" learning. On the contrary, human children do not learn following anything looking like that process, at least during their very first years. Babies develop and explore the world by themselves, focusing their interest on various activities driven both by internal motives and social guidance from adults who only have a folk understanding of their brains. Adults provide learning opportunities and scaffolding, but eventually young babies always decide for themselves what activity to practice or not. Specific tasks are rarely imposed to them. Yet, they steadily discover and learn how to use their body as well as its relationships with the physical and social environment. Also, the spectrum of skills that they learn continuously expands in an organized manner: they undergo a developmental trajectory in which simple skills are learnt first, and skills of progressively increasing complexity are subsequently learnt.

A link can be made to educational systems where research in several domains have tried to study how to provide a good learning experience to learners. This includes the experiences that allow better learning, and in which sequence they must be experienced. This problem is complementary to that of the learner that tries to learn efficiently, and the teacher here has to use as efficiently the limited time and motivational resources of the learner. Several results from psychology [112] and neuroscience [22] have argued that the human brain feels intrinsic pleasure in practicing activities of optimal difficulty or challenge. A teacher must exploit such activities to create positive psychological states of flow [124].

A grand challenge is thus to be able to build robotic machines that possess this capability to discover, adapt and develop continuously new know-how and new knowledge in unknown and changing environments, like human children. In 1950, Turing wrote that the child's brain would show us the way to intelligence: "Instead of trying to produce a program to simulate the adult mind, why not rather try to produce one which simulates the child's" [174]. Maybe, in opposition to work in the field of Artificial Intelligence who has focused on mechanisms trying to match the capabilities of "intelligent" human adults such as chess playing or natural language dialogue [134], it is time to take the advice of Turing seriously. This is what a new field, called developmental (or epigenetic) robotics, is trying to achieve [145] [178]. The approach of developmental robotics consists in importing and implementing concepts and mechanisms from developmental psychology [148], cognitive linguistics [123], and developmental cognitive neuroscience [139] where there has been a considerable amount of research and theories to understand and explain how children learn and develop. A number of general principles are underlying this research agenda: embodiment [116] [156], grounding [132], situatedness [105], self-organization [172] [158], enaction [176], and incremental learning [119].

Among the many issues and challenges of developmental robotics, two of them are of paramount importance: exploration mechanisms and mechanisms for abstracting and making sense of initially unknown sensorimotor channels. Indeed, the typical space of sensorimotor skills that can be encountered and learnt by a developmental robot, as those encountered by human infants, is immensely vast and inhomogeneous. With a sufficiently rich environment and multimodal set of sensors and effectors, the space of possible sensorimotor activities is simply too large to be explored exhaustively in any robot's life time: it is impossible to learn all possible skills and represent all conceivable sensory percepts. Moreover, some skills are very basic to learn, some other very complicated, and many of them require the mastery of others in order to be learnt. For example, learning to manipulate a piano toy requires first to know how to move one's hand to reach the piano and how to touch specific parts of the toy with the fingers. And knowing how to move the hand might require to know how to track it visually.

Exploring such a space of skills randomly is bound to fail or result at best on very inefficient learning [153]. Thus, exploration needs to be organized and guided. The approach of epigenetic robotics is to take inspiration from the mechanisms that allow human infants to be progressively guided, i.e. to develop. There are two broad classes of guiding mechanisms which control exploration:

1. **internal guiding mechanisms,** and in particular intrinsic motivation, responsible of spontaneous exploration and curiosity in humans, which is one of the central mechanisms investigated in FLOWERS, and technically amounts to achieve online active self-regulation of the growth of complexity in learning situations;
2. **social learning and guidance,** a learning mechanisms that exploits the knowledge of other agents in the environment and/or that is guided by those same agents. These mechanisms exist in many different forms like emotional reinforcement, stimulus enhancement, social motivation, guidance, feedback or imitation, some of which being also investigated in FLOWERS;

3.1.1. Internal guiding mechanisms

In infant development, one observes a progressive increase of the complexity of activities with an associated progressive increase of capabilities [148], children do not learn everything at one time: for example, they first learn to roll over, then to crawl and sit, and only when these skills are operational, they begin to learn how to stand. The perceptual system also gradually develops, increasing children perceptual capabilities other time while they engage in activities like throwing or manipulating objects. This make it possible to learn to identify objects in more and more complex situations and to learn more and more of their physical characteristics.

Development is therefore progressive and incremental, and this might be a crucial feature explaining the efficiency with which children explore and learn so fast. Taking inspiration from these observations, some roboticists and researchers in machine learning have argued that learning a given task could be made much easier for a robot if it followed a developmental sequence and "started simple" [108] [127]. However, in these experiments, the developmental sequence was crafted by hand: roboticists manually build simpler versions of a complex task and put the robot successively in versions of the task of increasing complexity. And when they wanted the robot to learn a new task, they had to design a novel reward function.

Thus, there is a need for mechanisms that allow the autonomous control and generation of the developmental trajectory. Psychologists have proposed that intrinsic motivations play a crucial role. Intrinsic motivations are mechanisms that push humans to explore activities or situations that have intermediate/optimal levels of novelty, cognitive dissonance, or challenge [112] [124] [126]. The role and structure of intrinsic motivation in humans have been made more precise thanks to recent discoveries in neuroscience showing the implication of dopaminergic circuits and in exploration behaviours and curiosity [125] [136] [166]. Based on this, a number of researchers have began in the past few years to build computational implementation of intrinsic motivation [153] [154] [164] [111] [137] [146] [165]. While initial models were developed for simple simulated worlds, a current challenge is to manage to build intrinsic motivation systems that can efficiently drive exploratory behaviour in high-dimensional unprepared real world robotic sensorimotor spaces [154], [153], [155], [163]. Specific and complex problems are posed by real sensorimotor spaces, in particular due to the fact that they are both high-dimensional as well as (usually) deeply inhomogeneous. As an example for the latter issue, some regions of real sensorimotor spaces are often unlearnable due to inherent stochasticity or difficulty, in which case heuristics based on the incentive to explore zones of maximal unpredictability or uncertainty, which are often used in the field of active learning [120] [133] typically lead to catastrophic results. The issue of high dimensionality does not only concern motor spaces, but also sensory spaces, leading to the problem of correctly identifying, among typically thousands of quantities, those latent variables that have links to behavioral choices. In FLOWERS, we aim at developing intrinsically motivated exploration mechanisms that scale in those spaces, by studying suitable abstraction processes in conjunction with exploration strategies.

3.1.2. Socially Guided and Interactive Learning

Social guidance is as important as intrinsic motivation in the cognitive development of human babies [148]. There is a vast literature on learning by demonstration in robots where the actions of humans in the environment are recognized and transferred to robots [107]. Most such approaches are completely passive: the human executes actions and the robot learns from the acquired data. Recently, the notion of interactive learning has been introduced in [173], [113], motivated by the various mechanisms that allow humans to socially guide a robot [160]. In an interactive context the steps of self-exploration and social guidances are not separated and a robot learns by self exploration and by receiving extra feedback from the social context [173], [142] [147].

Social guidance is also particularly important for learning to segment and categorize the perceptual space. Indeed, parents interact a lot with infants, for example teaching them to recognize and name objects or characteristics of these objects. Their role is particularly important in directing the infant attention towards objects of interest that will make it possible to simplify at first the perceptual space by pointing out a segment of the environment that can be isolated, named and acted upon. These interactions will then be complemented by the children own experiments on the objects chosen according to intrinsic motivation in order to improve the knowledge of the object, its physical properties and the actions that could be performed with it.

In FLOWERS, we are aiming at including intrinsic motivation system in the self-exploration part thus combining efficient self-learning with social guidance [150], [151]. We also work on developing perceptual capabilities by gradually segmenting the perceptual space and identifying objects and their characteristics through interaction with the user [32] and robots experiments [138]. Another challenge is to allow for more flexible interaction protocols with the user in terms of what type of feedback is provided and how it is provided [144].

Exploration mechanisms are combined with research in the following directions:

3.1.3. Cumulative learning, reinforcement learning and optimization of autonomous skill learning

FLOWERS develops machine learning algorithms that can allow embodied machines to acquire cumulatively sensorimotor skills. In particular, we develop optimization and reinforcement learning systems which allow robots to discover and learn dictionaries of motor primitives, and then combine them to form higher-level sensorimotor skills.

3.1.4. Autonomous perceptual and representation learning

In order to harness the complexity of perceptual and motor spaces, as well as to pave the way to higher-level cognitive skills, developmental learning requires abstraction mechanisms that can infer structural information out of sets of sensorimotor channels whose semantics is unknown, discovering for example the topology of the body or the sensorimotor contingencies (proprioceptive, visual and acoustic). This process is meant to be open- ended, progressing in continuous operation from initially simple representations towards abstract concepts and categories similar to those used by humans. Our work focuses on the study of various techniques for:

- autonomous multimodal dimensionality reduction and concept discovery;
- incremental discovery and learning of objects using vision and active exploration, as well as of auditory speech invariants;
- learning of dictionaries of motion primitives with combinatorial structures, in combination with linguistic description;
- active learning of visual descriptors useful for action (e.g. grasping);

3.1.5. Embodiment and maturational constraints

FLOWERS studies how adequate morphologies and materials (i.e. morphological computation), associated to relevant dynamical motor primitives, can importantly simplify the acquisition of apparently very complex skills such as full-body dynamic walking in biped. FLOWERS also studies maturational constraints, which are mechanisms that allow for the progressive and controlled release of new degrees of freedoms in the sensorimotor space of robots.

3.1.6. Discovering and abstracting the structure of sets of uninterpreted sensors and motors

FLOWERS studies mechanisms that allow a robot to infer structural information out of sets of sensorimotor channels whose semantics is unknown, for example the topology of the body and the sensorimotor contingencies (proprioceptive, visual and acoustic). This process is meant to be open-ended, progressing in continuous operation from initially simple representations to abstract concepts and categories similar to those used by humans.

GRAPHDECO Project-Team

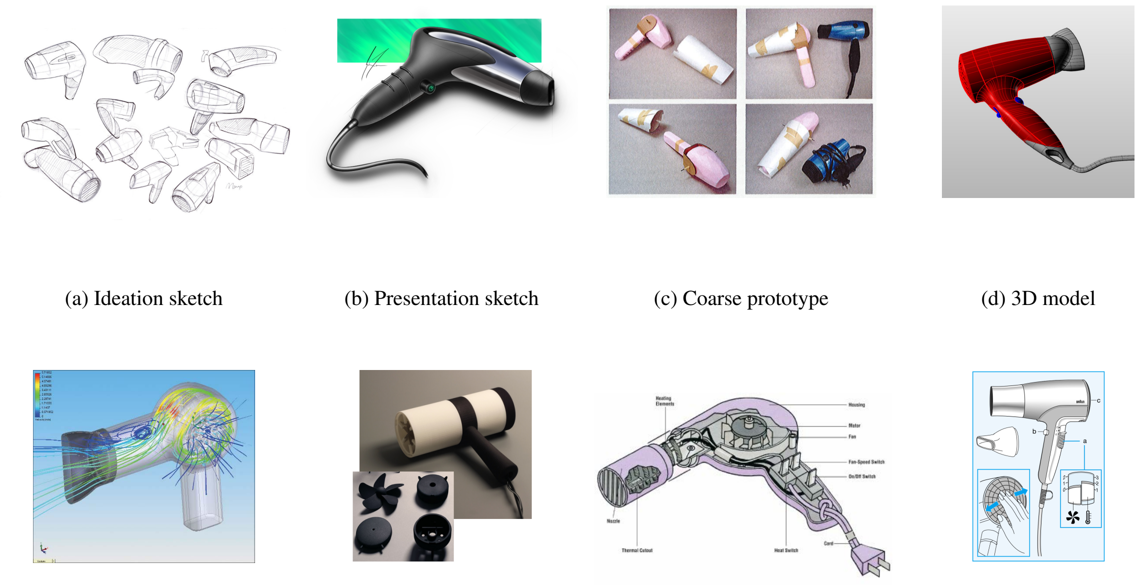
3. Research Program

3.1. Introduction

Our research program is oriented around two main axes: 1) Computer-Assisted Design with Heterogeneous Representations and 2) Graphics with Uncertainty and Heterogeneous Content. These two axes are governed by a set of common fundamental goals, share many common methodological tools and are deeply intertwined in the development of applications.

3.1.1. Computer-Assisted Design with Heterogeneous Representations

Designers use a variety of visual representations to explore and communicate about a concept. Figure 2 illustrates some typical representations, including sketches, hand-made prototypes, 3D models, 3D printed prototypes or instructions.



(a) Ideation sketch (b) Presentation sketch (c) Coarse prototype (d) 3D model

(f) Simulation (e) 3D Printing (g) Technical diagram (h) Instructions

Figure 2. Various representations of a hair dryer at different stages of the design process. Image source, in order: c-maeng on deviantart.com, shauntur on deviantart.com, "Prototyping and Modelmaking for Product Design" Hallgrimsson, B., Laurence King Publishers, 2012, samsher511 on turbosquid.com, my.solidworks.com, weilung tseng on cargocollective.com, howstuffworks.com, u-manual.com

The early representations of a concept, such as rough sketches and hand-made prototypes, help designers formulate their ideas and test the form and function of multiple design alternatives. These low-fidelity representations are meant to be cheap and fast to produce, to allow quick exploration of the *design space* of the concept. These representations are also often approximate to leave room for subjective interpretation and to stimulate imagination; in this sense, these representations can be considered *uncertain*. As the concept gets more finalized, time and effort are invested in the production of more detailed and accurate representations, such as high-fidelity 3D models suitable for simulation and fabrication. These detailed models can also be used to create didactic instructions for assembly and usage.

Producing these different representations of a concept requires specific skills in sketching, modeling, manufacturing and visual communication. For these reasons, professional studios often employ different experts to produce the different representations of the same concept, at the cost of extensive discussions and numerous iterations between the actors of this process. The complexity of the multi-disciplinary skills involved in the design process also hinders their adoption by laymen.

Existing solutions to facilitate design have focused on a subset of the representations used by designers. However, no solution considers all representations at once, for instance to directly convert a series of sketches into a set of physical prototypes. In addition, all existing methods assume that the concept is unique rather than ambiguous. As a result, rich information about the variability of the concept is lost during each conversion step.

We plan to facilitate design for professionals and laymen by adressing the following objectives:

- We want to assist designers in the exploration of the *design space* that captures the possible variations of a concept. By considering a concept as a *distribution* of shapes and functionalities rather than a single object, our goal is to help designers consider multiple design alternatives more quickly and effectively. Such a representation should also allow designers to preserve multiple alternatives along all steps of the design process rather than committing to a single solution early on and pay the price of this decision for all subsequent steps. We expect that preserving alternatives will facilitate communication with engineers, managers and clients, accelerate design iterations and even allow mass personalization by the end consumers.
- We want to support the various representations used by designers during concept development. While drawings and 3D models have received significant attention in past Computer Graphics research, we will also account for the various forms of rough physical prototypes made to evaluate the shape and functionality of a concept. Depending on the task at hand, our algorithms will either analyse these prototypes to generate a virtual concept, or assist the creation of these prototypes from a virtual model. We also want to develop methods capable of adapting to the different drawing and manufacturing techniques used to create sketches and prototypes. We envision design tools that conform to the habits of users rather than impose specific techniques to them.
- We want to make professional design techniques available to novices. Affordable software, hardware and online instructions are democratizing technology and design, allowing small businesses and individuals to compete with large companies. New manufacturing processes and online interfaces also allow customers to participate in the design of an object via mass personalization. However, similarly to what happened for desktop publishing thirty years ago, desktop manufacturing tools need to be simplified to account for the needs and skills of novice designers. We hope to support this trend by adapting the techniques of professionals and by automating the tasks that require significant expertise.

3.1.2. Graphics with Uncertainty and Heterogeneous Content

Our research is motivated by the observation that traditional CG algorithms have not been designed to account for uncertain data. For example, global illumination rendering assumes accurate virtual models of geometry, light and materials to simulate light transport. While these algorithms produce images of high realism, capturing effects such as shadows, reflections and interreflections, they are not applicable to the growing mass of uncertain data available nowadays.

The need to handle uncertainty in CG is timely and pressing, given the large number of *heterogeneous sources of 3D content* that have become available in recent years. These include data from cheap depth+image sensors (e.g., Kinect or the Tango), 3D reconstructions from image/video data, but also data from large 3D geometry databases, or casual 3D models created using simplified sketch-based modeling tools. Such alternate content has varying levels of *uncertainty* about the scene or objects being modelled. This includes uncertainty in geometry, but also in materials and/or lights – which are often not even available with such content. Since CG algorithms cannot be applied directly, visual effects artists spend hundreds of hours correcting inaccuracies and completing the captured data to make them useable in film and advertising.

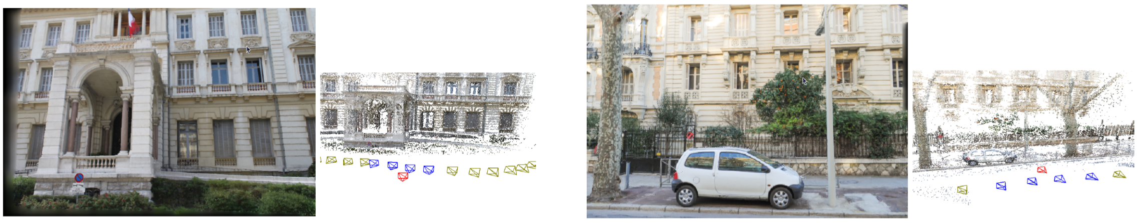


Figure 3. Image-Based Rendering (IBR) techniques use input photographs and approximate 3D to produce new synthetic views.

We identify a major scientific bottleneck which is the need to treat *heterogeneous* content, i.e., containing both (mostly captured) uncertain and perfect, traditional content. Our goal is to provide solutions to this bottleneck, by explicitly and formally modeling uncertainty in CG, and to develop new algorithms that are capable of mixed rendering for this content.

We strive to develop methods in which heterogeneous – and often uncertain – data can be handled automatically in CG with a principled methodology. Our main focus is on *rendering* in CG, including dynamic scenes (video/animations).

Given the above, we need to address the following challenges:

- Develop a theoretical model to handle uncertainty in computer graphics. We must define a new formalism that inherently incorporates uncertainty, and must be able to express traditional CG rendering, both physically accurate and approximate approaches. Most importantly, the new formulation must elegantly handle mixed rendering of perfect synthetic data and captured uncertain content. An important element of this goal is to incorporate *cost* in the choice of algorithm and the optimizations used to obtain results, e.g., preferring solutions which may be slightly less accurate, but cheaper in computation or memory.
- The development of rendering algorithms for heterogeneous content often requires preprocessing of image and video data, which sometimes also includes depth information. An example is the decomposition of images into intrinsic layers of reflectance and lighting, which is required to perform relighting. Such solutions are also useful as image-manipulation or computational photography techniques. The challenge will be to develop such “intermediate” algorithms for the uncertain and heterogeneous data we target.
- Develop efficient rendering algorithms for uncertain and heterogeneous content, reformulating rendering in a probabilistic setting where appropriate. Such methods should allow us to develop approximate rendering algorithms using our formulation in a well-grounded manner. The formalism should include probabilistic models of how the scene, the image and the data interact. These models should be data-driven, e.g., building on the abundance of online geometry and image databases, domain-driven, e.g., based on requirements of the rendering algorithms or perceptually guided, leading to plausible solutions based on limitations of perception.

GRAPHIK Project-Team

3. Research Program

3.1. Logic-based Knowledge Representation and Reasoning

We follow the mainstream *logic-based* approach to the KR domain. First-order logic (FOL) is the reference logic in KR and most formalisms in this area can be translated into fragments (i.e., particular subsets) of FOL. This is in particular the case for description logics and existential rules, two well-known KR formalisms studied in the team.

A large part of research in this domain can be seen as studying the *trade-off* between the expressivity of languages and the complexity of (sound and complete) reasoning in these languages. The fundamental problem in KR languages is entailment checking: is a given piece of knowledge entailed by other pieces of knowledge, for instance from a knowledge base (KB)? Another important problem is *consistency* checking: is a set of knowledge pieces (for instance the knowledge base itself) consistent, i.e., is it sure that nothing absurd can be entailed from it? The *ontology-mediated query answering* problem is a topical problem (see Section 3.3). It asks for the set of answers to a query in the KB. In the case of Boolean queries (i.e., queries with a yes/no answer), it can be recast as entailment checking.

3.2. Graph-based Knowledge Representation and Reasoning

Besides logical foundations, we are interested in KR formalisms that comply, or aim at complying with the following requirements: to have good *computational* properties and to allow users of knowledge-based systems to have a maximal *understanding and control* over each step of the knowledge base building process and use.

These two requirements are the core motivations for our graph-based approach to KR. We view labelled graphs as an *abstract representation* of knowledge that can be expressed in many KR languages (different kinds of conceptual graphs —historically our main focus—, the Semantic Web language RDF (Resource Description Framework), its extension RDFS (RDF Schema), expressive rules equivalent to the so-called tuple-generating-dependencies in databases, some description logics dedicated to query answering, etc.). For these languages, reasoning can be based on the structure of objects, thus based on graph-theoretic notions, while staying logically founded.

More precisely, our basic objects are labelled graphs (or hypergraphs) representing entities and relationships between these entities. These graphs have a natural translation in first-order logic. Our basic reasoning tool is graph homomorphism. The fundamental property is that graph homomorphism is sound and complete with respect to logical entailment *i.e.*, given two (labelled) graphs G and H, there is a homomorphism from G to H*if and only if* the formula assigned to G is entailed by the formula assigned to H. In other words, logical reasoning on these graphs can be performed by graph mechanisms. These knowledge constructs and the associated reasoning mechanisms can be extended (to represent rules for instance) while keeping this fundamental correspondence between graphs and logics.

3.3. Ontology-Mediated Query Answering

Querying knowledge bases has become a central problem in knowledge representation and in databases. A knowledge base (KB) is classically composed of a terminological part (metadata, ontology) and an assertional part (facts, data). Queries are supposed to be at least as expressive as the basic queries in databases, i.e., conjunctive queries, which can be seen as existentially closed conjunctions of atoms or as labelled graphs. The challenge is to define good trade-offs between the expressivity of the ontological language and the complexity of querying data in presence of ontological knowledge. Description logics have been so far the prominent family of formalisms for representing and reasoning with ontological knowledge. However, classical description logics were not designed for efficient data querying. On the other hand, database languages are able to process complex queries on huge databases, but without taking the ontology into account. There is thus a need for new languages and mechanisms, able to cope with the ever growing size of knowledge bases in the Semantic Web or in scientific domains.

This problem is related to two other problems identified as fundamental in KR:

- *Query-answering with incomplete information.* Incomplete information means that it might be unknown whether a given assertion is true or false. Databases classically make the so-called closed-world assumption: every fact that cannot be retrieved or inferred from the base is assumed to be false. Knowledge bases classically make the open-world assumption: if something cannot be inferred from the base, and neither can its negation, then its truth status is unknown. The need of coping with incomplete information is a distinctive feature of querying knowledge bases with respect to querying classical databases (however, as explained above, this distinction tends to disappear). The presence of incomplete information makes the query answering task much more difficult.
- *Reasoning with rules.* Researching types of rules and adequate manners to process them is a mainstream topic in the Semantic Web, and, more generally a crucial issue for knowledge-based systems. For several years, we have been studying some rules, both in their logical and their graph form, which are syntactically very simple but also very expressive. These rules, known as existential rules or Datalog+, can be seen as an abstraction of ontological knowledge expressed in the main languages used in the context of KB querying. See Section 6.1 for details on the results obtained.

A problem generalizing the above described problems, and particularly relevant in the context of multiple data/metadata sources, is *querying hybrid knowledge bases*. In a hybrid knowledge base, each component may have its own formalism and its own reasoning mechanisms. There may be a common ontology shared by all components, or each component may have its own ontology, with mappings being defined among the ontologies. The question is what kind of interactions between these components and/or what limitations on the languages preserve the decidability of basic problems and if so, a “reasonable”complexity. Note that there are strong connections with the issue of data integration in databases.

3.4. Imperfect Information and Priorities

While classical FOL is the kernel of many KR languages, to solve real-world problems we often need to consider features that cannot be expressed purely (or not naturally) in classical logic. The logic- and graph-based formalisms used for previous points have thus to be extended with such features.The following requirements have been identified from scenarios in decision making in the agronomy domain.

1. to cope with vague and uncertain information and preferences in queries;
2. to cope with multi-granularity knowledge;
3. to take into account different and potentially conflicting viewpoints ;
4. to integrate decision notions (priorities, gravity, risk, benefit);
5. to integrate argumentation-based reasoning.

Although the solutions we develop need to be validated on the applications that motivated them, we also want them to be sufficiently generic to be applied in other contexts. One angle of attack (but not the only possible one) consists in increasing the expressivity of our core languages, while trying to preserve their essential combinatorial properties, so that algorithmic optimizations can be transferred to these extensions.

HEPHAISTOS Project-Team

3. Research Program

3.1. Interval analysis

We are interested in real-valued system solving ($f(X)=0$, $f(X)\leq 0$), in optimization problems, and in the proof of the existence of properties (for example, it exists X such that $f(X)=0$ or it exist two values X_1, X_2 such that $f(X_1)>0$ and $f(X_2)<0$). There are few restrictions on the function f as we are able to manage explicit functions using classical mathematical operators (e.g. $\sin{(x+y)}+\log(\cos{(e^x)}+y^2)$ as well as implicit functions (e.g. determining if there are parameter values of a parametrized matrix such that the determinant of the matrix is negative, without calculating the analytical form of the determinant).

Solutions are searched within a finite domain (called a *box*) which may be either continuous or mixed (i.e. for which some variables must belong to a continuous range while other variables may only have values within a discrete set). An important point is that we aim at finding all the solutions within the domain whenever the computer arithmetic will allow it: in other words we are looking for *certified* solutions. For example, for 0-dimensional system solving, we will provide a box that contains one, and only one, solution together with a numerical approximation of this solution. This solution may further be refined at will using multi-precision.

The core of our methods is the use of *interval analysis* that allows one to manipulate mathematical expressions whose unknowns have interval values. A basic component of interval analysis is the *interval evaluation* of an expression. Given an analytical expression F in the unknowns $\{x_1,x_2,...,x_n\}$ and ranges $\{X_1,X_2,...,X_n\}$ for these unknowns we are able to compute a range $[A,B]$, called the interval evaluation, such that

$$\forall\{x_1,x_2,...,x_n\}\in\{X_1,X_2,...,X_n\}, A\leq F(x_1,x_2,...,x_n)\leq B \tag{92}$$

In other words the interval evaluation provides a lower bound of the minimum of F and an upper bound of its maximum over the box.

For example if $F=x\ sin(x+x^2)$ and $x\in[0.5,1.6]$, then $F([0.5,1.6])=[-1.362037441,1.6]$, meaning that for any x in [0.5,0.6] we guarantee that $-1.362037441\leq f(x)\leq 1.6$.

The interval evaluation of an expression has interesting properties:

- it can be implemented in such a way that the results are guaranteed with respect to round-off errors i.e. property 1 is still valid in spite of numerical errors induced by the use of floating point numbers
- if $A>0$ or $B<0$, then no values of the unknowns in their respective ranges can cancel F
- if $A>0$ ($B<0$), then F is positive (negative) for any value of the unknowns in their respective ranges

A major drawback of the interval evaluation is that $A(B)$ may be overestimated i.e. values of $x_1,x_2,...,x_n$ such that $F(x_1,x_2,...,x_n)=A(B)$ may not exist. This overestimation occurs because in our calculation each occurrence of a variable is considered as an independent variable. Hence if a variable has multiple occurrences, then an overestimation may occur. Such phenomena can be observed in the previous example where $B=1.6$ while the real maximum of F is approximately 0.9144. The value of B is obtained because we are using in our calculation the formula $F=xsin(y+z^2)$ with y,z having the same interval value than x.

Fortunately there are methods that allow one to reduce the overestimation and the overestimation amount decreases with the width of the ranges. The latter remark leads to the use of a branch-and-bound strategy in which for a given box a variable range will be bisected, thereby creating two new boxes that are stored in a list and processed later on. The algorithm is complete if all boxes in the list have been processed, or if during the process a box generates an answer to the problem at hand (e.g. if we want to prove that $F(X)<0$, then the algorithm stops as soon as $F(\mathcal{B})\geq 0$ for a certain box $\mathcal{B}$).

A generic interval analysis algorithm involves the following steps on the current box [1], [8], [5]:

1. *exclusion operators*: these operators determine that there is no solution to the problem within a given box. An important issue here is the extensive and smart use of the monotonicity of the functions
2. *filters*: these operators may reduce the size of the box i.e. decrease the width of the allowed ranges for the variables
3. *existence operators*: they allow one to determine the existence of a unique solution within a given box and are usually associated with a numerical scheme that allows for the computation of this solution in a safe way
4. *bisection*: choose one of the variable and bisect its range for creating two new boxes
5. *storage*: store the new boxes in the list

The scope of the HEPHAISTOS project is to address all these steps in order to find the most efficient procedures. Our efforts focus on mathematical developments (adapting classical theorems to interval analysis, proving interval analysis theorems), the use of symbolic computation and formal proofs (a symbolic pre-processing allows one to automatically adapt the solver to the structure of the problem), software implementation and experimental tests (for validation purposes).

Important note: We have insisted on interval analysis because this is a **major componant** or our robotics activity. Our theoretical work in robotics is an analysis of the robotic environment in order to exhibit proofs on the behavior of the system that may be qualitative (e.g. the proof that a cable-driven parallel robot with more than 6 non-deformable cables will have at most 6 cables under tension simultaneously) or quantitative. In the quantitative case as we are dealing with realistic and not toy examples (including our own prototypes that are developed whenever no equivalent hardware is available or to very our assumptions) we have to manage problems that are so complex that analytical solutions are probably out of reach (e.g. the direct kinematics of parallel robots) and we have to resort to algorithms and numerical analysis. We are aware of different approaches in numerical analysis (e.g. some team members were previously involved in teams devoted to computational geometry and algebraic geometry) but interval analysis provides us another approach with high flexibility, the possibility of managing non algebraic problems (e.g. the kinematics of cable-driven parallel robots with sagging cables, that involves inverse hyperbolic functions) and to address various types of issues (system solving, optimization, proof of existence ...).

3.2. Robotics

HEPHAISTOS, as a follow-up of COPRIN, has a long-standing tradition of robotics studies, especially for closed-loop robots [4], especially cable-driven parallel robots. We address theoretical issues with the purpose of obtaining analytical and theoretical solutions, but in many cases only numerical solutions can be obtained due to the complexity of the problem. This approach has motivated the use of interval analysis for two reasons:

1. the versatility of interval analysis allows us to address issues (e.g. singularity analysis) that cannot be tackled by any other method due to the size of the problem
2. uncertainties (which are inherent to a robotic device) have to be taken into account so that the *real* robot is guaranteed to have the same properties as the *theoretical* one, even in the worst case [15]. This is a crucial issue for many applications in robotics (e.g. medical or assistance robot)

Our field of study in robotics focuses on *kinematic* issues such as workspace and singularity analysis, positioning accuracy, trajectory planning, reliability, calibration, modularity management and, prominently, *appropriate design*, i.e. determining the dimensioning of a robot mechanical architecture that guarantees that the real robot satisfies a given set of requirements. The methods that we develop can be used for other robotic problems, see for example the management of uncertainties in aircraft design [6].

Our theoretical work must be validated through experiments that are essential for the sake of credibility. A contrario, experiments will feed theoretical work. Hence HEPHAISTOS works with partners on the development of real robots but also develops its own prototypes. In the last years we have developed a large number of prototypes and we have extended our development to devices that are not strictly robots but are part of an overall environment for assistance. We benefit here from the development of new miniature, low energy computers with an interface for analog and logical sensors such as the Arduino or the Phidgets. The web pages http://www-sop.inria.fr/hephaistos/mediatheque/index.html presents all of our prototypes and experimental work.

HYBRID Project-Team

3. Research Program

3.1. Research Program

The scientific objective of Hybrid team is to improve 3D interaction of one or multiple users with virtual environments, by making full use of physical engagement of the body, and by incorporating the mental states by means of brain-computer interfaces. We intend to improve each component of this framework individually, but we also want to improve the subsequent combinations of these components.

The "hybrid" 3D interaction loop between one or multiple users and a virtual environment is depicted in Figure 1 . Different kinds of 3D interaction situations are distinguished (red arrows, bottom): 1) body-based interaction, 2) mind-based interaction, 3) hybrid and/or 4) collaborative interaction (with at least two users). In each case, three scientific challenges arise which correspond to the three successive steps of the 3D interaction loop (blue squares, top): 1) the 3D interaction technique, 2) the modeling and simulation of the 3D scenario, and 3) the design of appropriate sensory feedback.

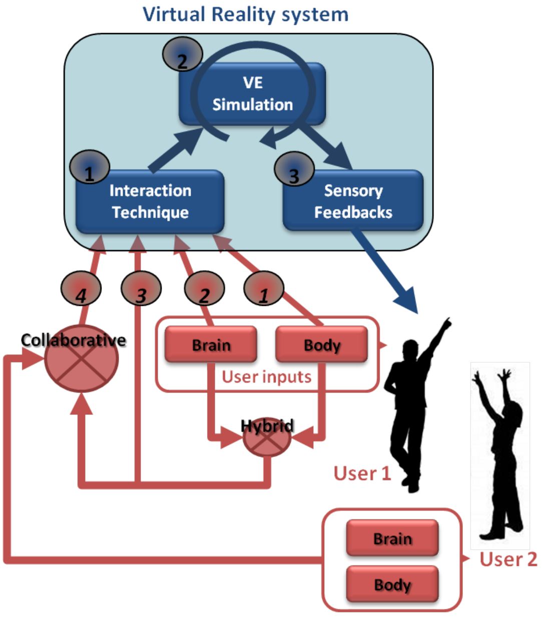


Figure 1. 3D hybrid interaction loop between one or multiple users and a virtual reality system. Top (in blue) three steps of 3D interaction with a virtual environment: (1-blue) interaction technique, (2-blue) simulation of the virtual environment, (3-blue) sensory feedbacks. Bottom (in red) different cases of interaction: (1-red) body-based, (2-red) mind-based, (3-red) hybrid, and (4-red) collaborative 3D interaction.

The 3D interaction loop involves various possible inputs from the user(s) and different kinds of output (or sensory feedback) from the simulated environment. Each user can involve his/her body and mind by means of corporal and/or brain-computer interfaces. A hybrid 3D interaction technique (1) mixes mental and motor inputs and translates them into a command for the virtual environment. The real-time simulation (2) of the virtual environment is taking into account these commands to change and update the state of the virtual world and virtual objects. The state changes are sent back to the user and perceived by means of different sensory feedbacks (e.g., visual, haptic and/or auditory) (3). The sensory feedbacks are closing the 3D interaction loop. Other users can also interact with the virtual environment using the same procedure, and can eventually "collaborate" by means of "collaborative interactive techniques" (4).

This description is stressing three major challenges which correspond to three mandatory steps when designing 3D interaction with virtual environments:

- **3D interaction techniques:** This first step consists in translating the actions or intentions of the user (inputs) into an explicit command for the virtual environment. In virtual reality, the classical tasks that require such kinds of user command were early categorized in four [38]: navigating the virtual world, selecting a virtual object, manipulating it, or controlling the application (entering text, activating options, etc). The addition of a third dimension, the use of stereoscopic rendering and the use of advanced VR interfaces make however inappropriate many techniques that proved efficient in 2D, and make it necessary to design specific interaction techniques and adapted tools. This challenge is here renewed by the various kinds of 3D interaction which are targeted. In our case, we consider various cases, with motor and/or cerebral inputs, and potentially multiple users.
- **Modeling and simulation of complex 3D scenarios:** This second step corresponds to the update of the state of the virtual environment, in real-time, in response to all the potential commands or actions sent by the user. The complexity of the data and phenomena involved in 3D scenarios is constantly increasing. It corresponds for instance to the multiple states of the entities present in the simulation (rigid, articulated, deformable, fluids, which can constitute both the user's virtual body and the different manipulated objects), and the multiple physical phenomena implied by natural human interactions (squeezing, breaking, melting, etc). The challenge consists here in modeling and simulating these complex 3D scenarios and meeting, at the same time, two strong constraints of virtual reality systems: performance (real-time and interactivity) and genericity (e.g., multi-resolution, multi-modal, multi-platform, etc).
- **Immersive sensory feedbacks:** This third step corresponds to the display of the multiple sensory feedbacks (output) coming from the various VR interfaces. These feedbacks enable the user to perceive the changes occurring in the virtual environment. They are closing the 3D interaction loop, making the user immersed, and potentially generating a subsequent feeling of presence. Among the various VR interfaces which have been developed so far we can stress two kinds of sensory feedback: visual feedback (3D stereoscopic images using projection-based systems such as CAVE systems or Head Mounted Displays); and haptic feedback (related to the sense of touch and to tactile or force-feedback devices). The Hybrid team has a strong expertize in haptic feedback, and in the design of haptic and "pseudo-haptic" rendering [41]. Note that a major trend in the community, which is strongly supported by the Hybrid team, relates to a "perception-based" approach, which aims at designing sensory feedbacks which are well in line with human perceptual capacities.

These three scientific challenges are addressed differently according to the context and the user inputs involved. We propose to consider three different contexts, which correspond to the three different research axes of the Hybrid research team, namely : 1) body-based interaction (motor input only), 2) mind-based interaction (cerebral input only), and then 3) hybrid and collaborative interaction (i.e., the mixing of body and brain inputs from one or multiple users).

3.2. Research Axes

The scientific activity of Hybrid team follows three main axes of research:

- **Body-based interaction in virtual reality.** Our first research axis concerns the design of immersive and effective "body-based" 3D interactions, i.e., relying on a physical engagement of the user's body. This trend is probably the most popular one in VR research at the moment. Most VR setups make use of tracking systems which measure specific positions or actions of the user in order to interact with a virtual environment. However, in recent years, novel options have emerged for measuring “full-body” movements or other, even less conventional, inputs (e.g. body equilibrium). In this first research axis we are thus concerned by the emergence of new kinds of “body-based interaction” with virtual environments. This implies the design of novel 3D user interfaces and novel 3D interactive techniques, novel simulation models and techniques, and novel sensory feedbacks for body-based interaction with virtual worlds. It involves real-time physical simulation of complex interactive phenomena, and the design of corresponding haptic and pseudo-haptic feedback.

- **Mind-based interaction in virtual reality.** Our second research axis concerns the design of immersive and effective “mind-based” 3D interactions in Virtual Reality. Mind-based interaction with virtual environments is making use of Brain-Computer Interface technology. This technology corresponds to the direct use of brain signals to send “mental commands” to an automated system such as a robot, a prosthesis, or a virtual environment. BCI is a rapidly growing area of research and several impressive prototypes are already available. However, the emergence of such a novel user input is also calling for novel and dedicated 3D user interfaces. This implies to study the extension of the mental vocabulary available for 3D interaction with VE, then the design of specific 3D interaction techniques "driven by the mind" and, last, the design of immersive sensory feedbacks that could help improving the learning of brain control in VR.
- **Hybrid and collaborative 3D interaction.** Our third research axis intends to study the combination of motor and mental inputs in VR, for one or multiple users. This concerns the design of mixed systems, with potentially collaborative scenarios involving multiple users, and thus, multiple bodies and multiple brains sharing the same VE. This research axis therefore involves two interdependent topics: 1) collaborative virtual environments, and 2) hybrid interaction. It should end up with collaborative virtual environments with multiple users, and shared systems with body and mind inputs.

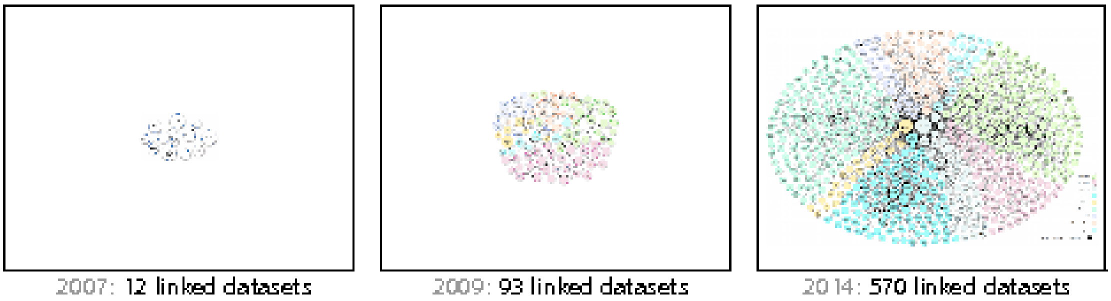
ILDA Project-Team

3. Research Program

3.1. Introduction

Our ability to acquire or generate, store, process, interlink and query data has increased spectacularly over the last few years. The corresponding advances are commonly grouped under the umbrella of so called *Big Data*. Even if the latter has become a buzzword, these advances are real, and they are having a profound impact in domains as varied as scientific research, commerce, social media, industrial processes or e-government. Yet, looking ahead, emerging technologies related to what we now call the *Web of Data* (a.k.a the Semantic Web) have the potential to create an even larger revolution in data-driven activities, by making information accessible to machines as semistructured data [28] that eventually becomes actionable knowledge. Indeed, novel Web data models considerably ease the interlinking of semi-structured data originating from multiple independent sources. They make it possible to associate machine-processable semantics with the data. This in turn means that heterogeneous systems can exchange data, infer new data using reasoning engines, and that software agents can cross data sources, resolving ambiguities and conflicts between them [71]. Datasets are becoming very rich and very large. They are gradually being made even larger and more heterogeneous, but also much more useful, by interlinking them, as exemplified by the Linked Data initiative [47].

These advances raise research questions and technological challenges that span numerous fields of computer science research: databases, communication networks, security and trust, data mining, as well as human-computer interaction. Our research is based on the conviction that interactive systems play a central role in many data-driven activity domains. Indeed, no matter how elaborate the data acquisition, processing and storage pipelines are, data eventually get processed or consumed one way or another by users. The latter are faced with large, increasingly interlinked heterogeneous datasets (see, e.g., Figure 1) that are organized according to complex structures, resulting in overwhelming amounts of both raw data and structured information. Users thus require effective tools to make sense of their data and manipulate them.


2007: 12 linked datasets

2009: 93 linked datasets

2014: 570 linked datasets

Figure 1. Linking Open Data cloud diagram from 2007 to 2014 – http://lod-cloud.net

We approach this problem from the perspective of the Human-Computer Interaction (HCI) field of research, whose goal is to study how humans interact with computers and inspire novel hardware and software designs aimed at optimizing properties such as efficiency, ease of use and learnability, in single-user or cooperative work contexts. More formally, HCI is about designing systems that lower the barrier between users' cognitive model of what they want to accomplish, and computers' understanding of this model. HCI is about the design, implementation and evaluation of computing systems that humans interact with [52], [73]. It is a highly multidisciplinary field, with experts from computer science, cognitive psychology, design, engineering, ethnography, human factors and sociology.

In this broad context, ILDA aims at designing interactive systems that display [37], [59], [80] the data and let users interact with them, aiming to help users better *navigate* and *comprehend* large webs of data represented visually, as well as *relate* and *manipulate* them.

Our research agenda consists of the three complementary axes detailed in the following subsections. Designing systems that consider interaction in close conjunction with data semantics is pivotal to all three axes. Those semantics will help drive navigation in, and manipulation of, the data, so as to optimize the communication bandwidth between users and data.

3.2. Semantics-driven Data Manipulation

Participants: Emmanuel Pietriga, Caroline Appert, Hande Ozaygen, Hugo Romat.

The Web of Data has been maturing for the last fifteen years and is starting to gain adoption across numerous application domains (Figure 1). Now that most foundational building blocks are in place, from knowledge representation, inference mechanisms and query languages [48], all the way up to the expression of data presentation knowledge [66] and to mechanisms like look-up services [79] or spreading activation [43], we need to pay significant attention to how human beings are going to interact with this new Web, if it is to *"reach its full potential"* [44].

Most efforts in terms of user interface design and development for the Web of data have essentially focused on tools for software developers or subject-matter experts who create ontologies and populate them [54], [42]. Tools more oriented towards end-users are starting to appear [34], [36], [49], [50], [53], [61], including the so-called *linked data browsers* [47]. However, those browsers are in most cases based on quite conventional point-and-click hypertext interfaces that present data to users in a very page-centric, web-of-documents manner that is ill-suited to navigating in, and manipulating, webs of data.

To be successful, interaction paradigms that let users navigate and manipulate data on the Web have to be tailored to the radically different way of browsing information enabled by it, where users directly interact with the data rather than with monolithic documents. The general research question addressed in this part of our research program is how to design novel interaction techniques that help users manipulate their data more efficiently. By data manipulation, we mean all low-level tasks related to manually creating new content, modifying and cleaning existing content, merging data from different sources, establishing connections between datasets, categorizing data, and eventually sharing the end results with other users; tasks that are currently considered quite tedious because of the sheer complexity of the concepts, data models and syntax, and the interplay between all of them.

Our approach is based on the conviction that there is a strong potential for cross-fertilization, as mentioned earlier: on the one hand, user interface design is essential to the management and understanding of webs of data; on the other hand, interlinked datasets enriched with even a small amount of semantics can help create more powerful user interfaces, that provide users with the right information at the right time.

We envision systems that focus on the data themselves, exploiting the underlying *semantics and structure* in the background rather than exposing them – which is what current user interfaces for the Web of Data often do. We envision interactive systems in which the semantics and structure are not exposed directly to users, but serve as input to the system to generate interactive representations that convey information relevant to the task at hand and best afford the possible manipulation actions.

3.3. Generalized Multi-scale Navigation

Participants: Olivier Chapuis, Emmanuel Pietriga, Caroline Appert, Anastasia Bezerianos, Olivier Gladin, Anna Gogolou, Maria Jesus Lobo Gunther, Arnaud Prouzeau.

The foundational question addressed here is what to display when, where and how, so as to provide effective support to users in their data understanding and manipulation tasks. ILDA targets contexts in which workers have to interact with complementary views on the same data, or with views on different-but-related datasets, possibly at different levels of abstraction. Being able to combine or switch between representations of the data at different levels of detail and merge data from multiple sources in a single representation is central to many scenarios. This is especially true in both of the application domains we consider: mission-critical systems (e.g., natural disaster crisis management) and the exploratory analysis of scientific data (e.g., correlate theories and heterogeneous observational data for an analysis of a given celestial body in Astrophysics).

A significant part of our research over the last ten years has focused on multi-scale interfaces. We designed and evaluated novel interaction techniques, but also worked actively on the development of open-source UI toolkits for multi-scale interfaces (see Section 6.2). These interfaces let users navigate large but relatively homogeneous datasets at different levels of detail, on both workstations [69], [31], [65], [64], [63], [32], [68], [30], [70] and wall-sized displays [5], [55], [67], [60], [33], [39], [38]. This part of the ILDA research program is about extending multi-scale navigation in two directions: 1. Enabling the representation of multiple, spatially-registered but widely varying, multi-scale data layers in Geographical Information Systems (GIS); 2. Generalizing the multi-scale navigation paradigm to interconnected, heterogeneous datasets as found on the Web of Data.

The first research problem is mainly investigated in collaboration with IGN in the context of ANR project MapMuxing (Section 9.2.1), which stands for *multi-dimensional map multiplexing*. Project MapMuxing aims at going beyond the traditional pan & zoom and overview+detail interface schemes, and at designing and evaluating novel cartographic visualizations that rely on high-quality generalization, *i.e.*, the simplification of geographic data to make it legible at a given map scale [76], [77], and symbol specification. Beyond project MapMuxing, we are also investigating multi-scale multiplexing techniques for geo-localized data in the specific context of ultra-high-resolution wall-sized displays, where the combination of a very high pixel density and large physical surface (Figure 2) enable us to explore designs that involve collaborative interaction and physical navigation in front of the workspace. This is work done in cooperation with team Massive Data at Inria Chile.

The second research problem is about the extension of multi-scale navigation to interconnected, heterogeneous datasets. Generalization has a rather straightforward definition in the specific domain of geographical information systems, where data items are geographical entities that naturally aggregate as scale increases. But it is unclear how generalization could work for representations of the more heterogeneous webs of data that we consider in the first axis of our research program. Those data form complex networks of resources with multiple and quite varied relationships between them, that cannot rely on a single, unified type of representation (a role played by maps in GIS applications).

Addressing the limits of current generalization processes is a longer-term, more exploratory endeavor. Here again, the machine-processable semantics and structure of the data give us an opportunity to rethink how users navigate interconnected heterogeneous datasets. Using these additional data, we investigate ways to generalize the multi-scale navigation paradigm to datasets whose layout and spatial relationships can be much richer and much more diverse than what can be encoded with static linear hierarchies as typically found today in interfaces for browsing maps or large imagery. Our goal is thus to design and develop highly dynamic and versatile multi-scale information spaces for heterogeneous data whose structure and semantics are not known in advance, but discovered incrementally.

3.4. Novel Forms of Input for Groups and Individuals

Participants: Caroline Appert, Anastasia Bezerianos, Olivier Chapuis, Emmanuel Pietriga, André Spritzer, Rafael Morales Gonzalez, Bruno Fruchard.

Analyzing and manipulating large datasets can involve multiple users working together in a coordinated manner in multi-display environments: workstations, handheld devices, wall-sized displays [33]. Those users work towards a common goal, navigating and manipulating data displayed on various hardware surfaces in a coordinated manner. Group awareness [46], [27] is central in these situations, as users, who may or may not be co-located in the same room, can have an optimal individual behavior only if they have a clear picture of what their collaborators have done and are currently doing in the global context. We work on the design and implementation of interactive systems that improve group awareness in co-located situations [56], making individual users able to figure out what other users are doing without breaking the flow of their own actions.

In addition, users need a rich interaction vocabulary to handle large, structured datasets in a flexible and powerful way, regardless of the context of work. Input devices such as mice and trackpads provide a limited number of input actions, thus requiring users to switch between modes to perform different types of data manipulation and navigation actions. The action semantics of these input devices are also often too much dependent on the display output. For instance, a mouse movement and click can only be interpreted according to the graphical controller (widget) above which it is moved. We focus on designing powerful input techniques based upon technologies such as tactile surfaces (supported by UI toolkits developed in-house), 3D motion tracking systems, or custom-built controllers [58] *to complement (rather than replace) traditional input devices* such as keyboards, that remain the best method so far for text entry, and indirect input devices such as mice or trackpads for pixel-precise pointing actions.

The input vocabularies we investigate enable users to navigate and manipulate large and structured datasets in environments that involve multiple users and displays that vary in their size, position and orientation [33], [45], each having their own characteristics and affordances: wall displays [5], [81], workstations, tabletops [62], [41], tablets [6], [78], smartphones [10], [40], [74], [75], and combinations thereof [2], [9], [60], [33].

We aim at designing rich interaction vocabularies that go far beyond what current touch interfaces offer, which rarely exceeds five gestures such as simple slides and pinches. Designing larger gesture vocabularies requires identifying discriminating dimensions (e.g., the presence or absence of anchor points and the distinction between internal and external frames of reference [6]) in order to structure a space of gestures that interface designers can use as a dictionary for choosing a coherent set of controls. These dimensions should be few and simple, so as to provide users with gestures that are easy to memorize and execute. Beyond gesture complexity, the scalability of vocabularies also depends on our ability to design robust gesture recognizers that will allow users to fluidly chain simple gestures that make it possible to interlace navigation and manipulation actions.

We also plan to study how to further extend input vocabularies by combining touch [10], [6], [62] and mid-air gestures [5] with physical objects [51], [72], [58] and classical input devices such as keyboards to enable users to input commands to the system or to involve other users in their workflow (request for help, delegation, communication of personal findings, etc.) [35], [57]. Gestures and objects encode a lot of information in their shape, dynamics and direction, that can be directly interpreted in relation with the user, independently from the display output. Physical objects can also greatly improve coordination among actors for, e.g., handling priorities or assigning specific roles.

IMAGINE Project-Team

3. Research Program

3.1. Methodology

As already stressed, thinking of future digital modeling technologies as an Expressive Virtual Pen enabling to seamlessly design, refine and convey animated 3D content, leads to revisit models for shapes, motions and stories from a user-centered perspective. More specifically, inspiring from the user-centered interfaces developed in the Human Computer Interaction domain, we introduced the new concept of user-centered graphical models. Ideally, such models should be designed to behave, under any user action, the way a human user would have predicted. In our case, user's actions may include creation gestures such as sketching to draft a shape or direct a motion, deformation gestures such as stretching a shape in space or a motion in time, or copy-paste gestures to transfer some of the features from existing models to other ones. User-centered graphical models need to incorporate knowledge in order to seamlessly generate the appropriate content from such actions. We are using the following methodology to advance towards these goals:

- Develop high-level models for shapes, motion and stories that embed the necessary knowledge to respond as expected to user actions. These models should provide the appropriate handles for conveying the user's intent while embedding procedural methods that seamlessly take care of the appropriate details and constraints.
- Combine these models with expressive design and control tools such as gesture-based control through sketching, sculpting, or acting, towards interactive environments where users can create a new virtual scene, play with it, edit or refine it, and semi-automatically convey it through a video.

3.2. Validation

Validation is a major challenge when developing digital creation tools: there is no ideal result to compare with, in contrast with more standard problems such as reconstructing existing shapes or motions. Therefore, we had to think ahead about our validation strategy: new models for geometry or animation can be validated, as usually done in Computer Graphics, by showing that they solve a problem never tackled before or that they provide a more general or more efficient solution than previous methods. The interaction methods we are developing for content creation and editing rely as much as possible on existing interaction design principles already validated within the HCI community. We also occasionally develop new interaction tools, most often in collaboration with this community, and validate them through user studies. Lastly, we work with expert users from various application domains through our collaborations with professional artists, scientists from other domains, and industrial partners: these expert users validate the use of our new tools compared to their usual pipeline.

3.3. Application Domains

This research can be applied to any situation where users need to create new, imaginary, 3D content. Our work should be instrumental, in the long term, for the visual arts, from the creation of 3D films and games to the development of new digital planning tools for theater or cinema directors. Our models can also be used in interactive prototyping environments for engineering. They can help promoting interactive digital design to scientists, as a tool to quickly express, test and refine models, as well as an efficient way for conveying them to other people. Lastly, we expect our new methodology to put digital modeling within the reach of the general public, enabling educators, media and other practitioners to author their own 3D content.

Our current application domains are:

- Visual arts
  - Modeling and animation for 3D films and games.
  - Virtual cinematography and tools for theater directors.
- Engineering
  - Industrial design.
  - Mechanical & civil engineering.
- Natural Sciences
  - Virtual functional anatomy.
  - Virtual plants.
- Education and Creative tools
  - Sketch-based teaching.
  - Creative environments for novice users.

The diversity of users these domains bring, from digital experts to other professionals and novices, gives us excellent opportunities to validate our general methodology with different categories of users. Our ongoing projects in these various application domains are listed in Section 6.

LACODAM Team

3. Research Program

3.1. Introduction

The three research axes of the Lacodam project-team are the following. First, we briefly introduce these axes, as well as their interplay:

- The first research axis is dedicated to the design of *novel pattern mining methods*. Pattern mining is one of the most important approaches to discover novel knowledge in data, and one of our strongest areas of expertise. Work in this axis will be the most fundamental of all three axes, and is expected to serve as foundations for work on the other two axes.
- The second axis tackles another aspect of knowledge discovery in data: the *interaction between the user and the system*, in order to co-discover novel knowledge. Our team has a long experience to collaborate with domain experts, and is thus especially aware of the need to improve such interaction.
- The third axis concerns *decision support*. With the help of methods from the two previous axes, our goal here is to design systems that can either help humans to take better decisions in precise applicative contexts, or to allow machines to automatically take relevant decisions in situations where extremely fast reaction time is required.

The following figure sums up the detailed work presented in the next few pages: on the sides are the three research axes of the team (X-axis) and our main applications areas (Y-axis). In the middle are colored squares that represent the precise research topics of the team that will be described in this section, placed relatively to their axis and main application area. Lines represent projects that can link several topics, and that are also connected to their main application area.

3.2. Pattern mining algorithms

Twenty years of research in pattern mining have resulted in efficient approaches to handle the algorithmic complexity of the problem. Existing algorithms are now able to efficiently extract patterns with complex structures (ex: sequences, graphs, co-variations) from large datasets. However, when dealing with large, real world datasets, these methods still output a huge set of patterns, which is impractical for human analysis. This problem is called pattern explosion. The ongoing challenge of pattern mining research is to extract fewer but more meaningful patterns. The Lacodam team is committed to solve the pattern explosion problem following four research topics:

- the design of dedicated algorithms for mining temporal patterns
- the design of flexible pattern mining approaches
- the selection of interesting data mining results
- the design of parallel pattern algorithms to ensure scalability

The originality of our contributions relies on the exploration of knowledge-based approaches whose principle is to incorporate dedicated domain knowledge (aka application background knowledge) deep into the mining process. While most of the data mining approaches are based on agnostic approaches that are designed to cope with the pattern explosion, we propose to develop data mining techniques relying on knowledge-based artificial intelligence techniques. This covers the use of structured knowledge representations, as well as reasoning methods, in combination with mining.

The first approach concerns the classical approach of pattern mining which consists in using expert knowledge to define new pattern types (and related algorithms) that can solve applicative issues. In particular, we investigate how to handle temporality in pattern representations which turns out to be important in many real world applications (in particular for decision support) and deserves particular attention.

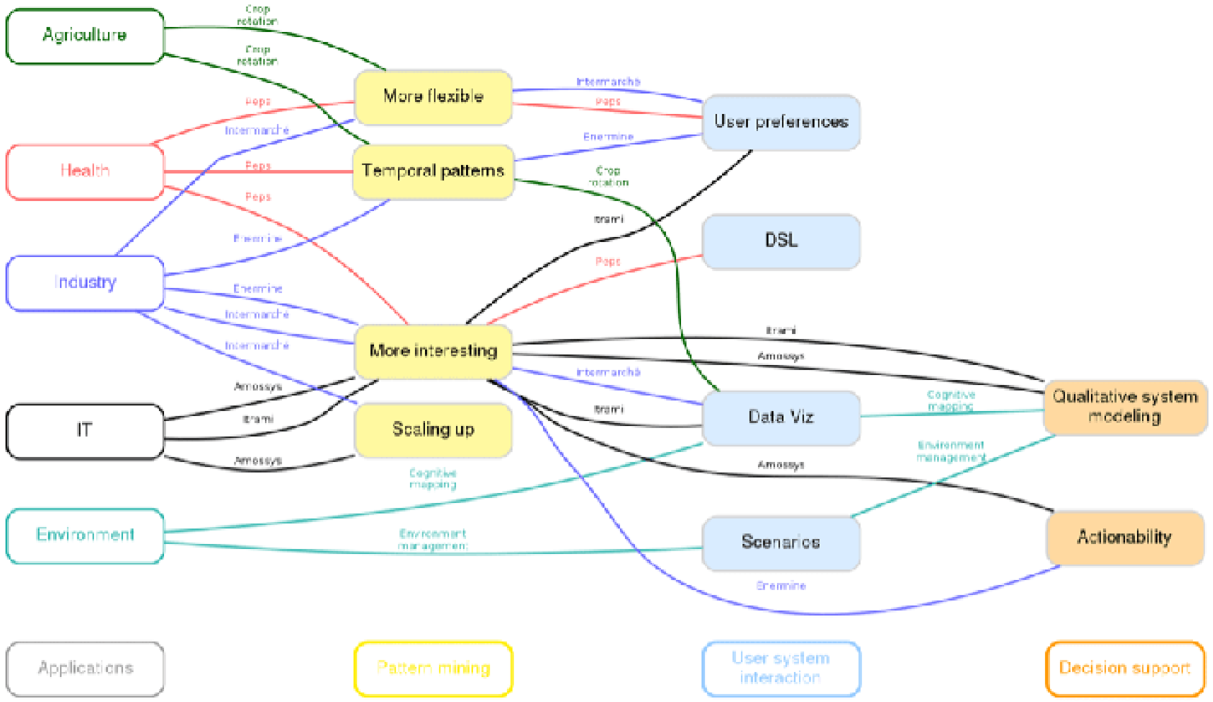


Figure 1. Lacodam research topics organized by axis and application

The two other approaches aim at proposing alternative pattern mining methods to let the user incorporate, by her own, knowledge that will help define her pattern domain of interest. Flexible pattern mining approaches enable analysts to easily incorporate extra knowledge, for example domain related constraints, in order to extract only the most relevant patterns. On the other hand, the selection of interesting data mining results aims at devising strategies to filter out the results that are useless for the data analyst. Beside the challenge related to algorithmic efficiency of such approaches, we are interested in formalizing the foundations of interestingness, according to background knowledge modeled with logic knowledge representation paradigms.

Last, pattern mining algorithms are computation-intensive, it is thus important to exploit all the available computing power. Parallelism is for a foreseeable future one of the main ways to speed up computations, and we have a strong competence on the design of parallel pattern mining algorithms. We will exploit this competence in order to guarantee that our approaches scale up to the real data provided by our partners.

3.3. User/system interaction

As we pointed out before, there is a strong need to present relevant patterns to the user. This can be done by using more specific constraints, background knowledge and/or tailor-made optimization functions. Due to the difficulty of determining these elements beforehand, one of the most promising solutions is that the system and the user co-construct the definition of most relevant patterns, i.e., to have a human in the loop. This requires to have means to present intermediate results to the user, and to get user feedback in order to guide the search space exploration process in the right direction. This is an important research axis for Lacodam, which will be tackled in several complementary ways:

- Domain Specific Languages: one way to interact with the user is to propose a Domain Specific Language (DSL) tailored to the domain at hand and to the analysis tasks to perform. The challenge is to propose a DSL allowing the users to easily express the required processing workflows, to deploy those workflows for mining large volumes of data and to offer as much automation as possible.
- What if / What for scenarios: we are also investigating the use of scenarios to query results from data mining processes, as well as other complex processes such as complex system simulations or model predictions. Such scenarios are answers to questions of the type “what if [situation]” or “what [should be done] for [expected outcome]”.
- User preferences: in exploratory analysis, users often do not have a precise enough idea of what they want, and are not able to formulate such queries. Lacodam is thus investigating simple ways for letting users express their interests and preferences, either during the mining process to guide the search space exploration, or after, to help in getting the most relevant results.
- Data visualization: most of the research directions presented in this document require users to examine patterns at some point. The output of most pattern mining algorithms is simply a (long) list of patterns. While this presentation can be sufficient in some applications, it is often not enough to provide a complete understanding, especially for non-experts in pattern mining. A transversal research topic that we want to develop in Lacodam is to propose data visualization techniques adequate to understanding output results. Numerous (failed) experiments have shown that data mining and data visualization are fields which require distinct skills, where researchers in one field usually do not make significant advances in the other field (this is detailed in [Keim 2010]). Thus, our strategy is to establish collaborations with prominent data visualization teams for this line of research, with a long term goal to recruit a specialist in data visualization if the opportunity arises.

3.4. Decision support

Patterns, especially predictive sequential patterns, resulting from mining a dataset have often a direct application in diagnosis. Lacodam inherits from the former Dream team a strong background in decision support systems, with an internationally recognized expertise in diagnosis. This AI subfield is concerned with determining if a system is operating normally or not, and if the system is in an abnormal state, to determine the cause of the faulty behavior. The considered system can as well be an agro- or eco-system, a software system or an animal or human being, as well.

The increasing volumes of data coming from a wide range of different systems (ex: sensor data from agro-environmental systems, log data from software systems, biological data coming from health monitoring systems) show that it is possible to gather more and more observations for such systems. Thus, it should be possible to exploit such observations to help human or software agents to take better decisions. Hence, while keeping the strong interest on decision support (and especially diagnosis) that existed in Dream, Lacodam adds the idea that the decision support systems should take advantage of the huge volumes of data available. This third and last research axis is thus a meeting point for all members of the team, as it requires to integrate AI techniques of traditional decision support systems with results from data mining techniques.

Two main research axes are investigated in Lacodam:

- Diagnosis-based approaches. We are exploring how to integrate knowledge found from pattern mining approaches, possibly with the help of interactive methods, into the qualitative models. The goal of such work is to partly automate the construction of the model, which can require a lot of human effort otherwise.
- Actionable patterns and rules. In many settings of “exploratory data mining”, the actual interest of a pattern is hard to assess, as it may be hard to measure or may be subjective (resulting from introducing the user in the mining process). However, there exist applications where once patterns are found, there are well defined measures to define what this pattern will bring to the user. Further, patterns and rules that can lead to actual actions beneficial to the user are called actionable patterns. Such actionable patterns and rules are especially important for industry.

3.5. Long-term goals

The following perspectives are at the convergence of the three research axes presented before, and can be seen as the ideal towards which our efforts tend:

- Automating data science workflow discovery. The current methods for extracting knowledge from data and building decision support systems require a lot of human effort. Our three research axes aim at alleviating this effort, by devising methods that are more generic and by improving the interaction between the user and the system. An ideal solution would be that the user could forget completely about the existence of pattern mining or decision support methods. Instead the user would only loosely specify her problem, while the system would construct for her various data science / decision support workflows, possibly further refined via interactions.

  We consider that this is a second order AI task, where AI techniques such as planning are used to explore the workflow search space, the workflow itself being composed of data mining and/or decision support components. This is a strategic evolution for data science endeavors, were the demand far exceeds the available human skilled manpower.
- Logic argumentation based on epistemic interest. Having increasingly automated approaches will require better and better ways to handle the interactions with the user. Our second long term goal is to explore the use of logic argumentation as an interaction tool between users and a data analysis tool. Alongside visualization and interactive data mining tools, it can be a way for users to query in an intuitive manner both the results and the way they were obtained. Such querying can also help the expert to reformulate her query in an interactive analysis setting.

  This research direction continues the work on “epistemic interest” presented before. Its goal is to exploit principles of interactive data analysis in the context of epistemic interest measures. Logic argumentation [Besnard 2014] can be a natural tool for interactions between the user and the system: display of possibly exhaustive list of arguments, relationships – whether reinforcement, compatibility or conflict – between arguments, variable degrees of arguments, and possible solutions for argument conflicts.

The first step is to define a formal argumentation framework for explaining data mining results. This implies to continue theoretical work on the foundations of argumentation in order to identify the most adapted framework (either existing or a new one to be defined). Logic argumentation may be implemented and deeply explored in ASP, allowing us to build on our expertise in this logic language.

- Collaborative feedback and knowledge management. We are convinced that improving the data science process, and possibly automating it, will rely at some point in the near future on the vast feedback that can be obtained by communities of user seamlessly collaborating over the web. Consider for example what has been achieved by collaborative platforms such as StackOverflow: it has become the reference site for any programming question.

  Data science is a more complex problem than programming, as in order to get help from the community, the user has to share her data and workflow, or at least some parts of them. This raises obvious privacy issues that may prevent this idea to succeed. As our research on automating the production of data science workflows should enable more people to have access to data science results, we are interested to investigate the design of collaborative platforms to exchange expert advices over data, workflows and analysis results, with an aim at exploiting this human feedback to improve the automated system with machine learning.

LAGADIC Project-Team

3. Research Program

3.1. Visual servoing

Basically, visual servoing techniques consist in using the data provided by one or several cameras in order to control the motions of a dynamic system [1]. Such systems are usually robot arms, or mobile robots, but can also be virtual robots, or even a virtual camera. A large variety of positioning tasks, or mobile target tracking, can be implemented by controlling from one to all the degrees of freedom of the system. Whatever the sensor configuration, which can vary from one on-board camera on the robot end-effector to several free-standing cameras, a set of visual features has to be selected at best from the image measurements available, allowing to control the desired degrees of freedom. A control law has also to be designed so that these visual features $\mathbf{s}(t)$ reach a desired value $\mathbf{s}^*$, defining a correct realization of the task. A desired planned trajectory $\mathbf{s}^*(t)$ can also be tracked. The control principle is thus to regulate the error vector $\mathbf{s}(t) - \mathbf{s}^*(t)$ to zero. With a vision sensor providing 2D measurements, potential visual features are numerous, since 2D data (coordinates of feature points in the image, moments, ...) as well as 3D data provided by a localization algorithm exploiting the extracted 2D features can be considered. It is also possible to combine 2D and 3D visual features to take the advantages of each approach while avoiding their respective drawbacks.

More precisely, a set $\mathbf{s}$ of k visual features can be taken into account in a visual servoing scheme if it can be written:

$$\mathbf{s} = \mathbf{s}(\mathbf{x}(\mathbf{p}(t)), \mathbf{a}) \tag{93}$$

where $\mathbf{p}(t)$ describes the pose at the instant t between the camera frame and the target frame, $\mathbf{x}$ the image measurements, and $\mathbf{a}$ a set of parameters encoding a potential additional knowledge, if available (such as for instance a coarse approximation of the camera calibration parameters, or the 3D model of the target in some cases).

The time variation of $\mathbf{s}$ can be linked to the relative instantaneous velocity $\mathbf{v}$ between the camera and the scene:

$$\dot{\mathbf{s}} = \frac{\partial \mathbf{s}}{\partial \mathbf{p}} \, \dot{\mathbf{p}} = \mathbf{L_s} \, \mathbf{v} \tag{94}$$

where $\mathbf{L_s}$ is the interaction matrix related to $\mathbf{s}$. This interaction matrix plays an essential role. Indeed, if we consider for instance an eye-in-hand system and the camera velocity as input of the robot controller, we obtain when the control law is designed to try to obtain an exponential decoupled decrease of the error:

$$\mathbf{v}_c = -\lambda \widehat{\mathbf{L_s}}^{+} (\mathbf{s} - \mathbf{s}^*) - \widehat{\mathbf{L_s}}^{+} \widehat{\frac{\partial \mathbf{s}}{\partial t}} \tag{95}$$

where λ is a proportional gain that has to be tuned to minimize the time-to-convergence, $\widehat{\mathbf{L_s}}^{+}$ is the pseudo-inverse of a model or an approximation of the interaction matrix, and $\widehat{\frac{\partial \mathbf{s}}{\partial t}}$ an estimation of the features velocity due to a possible own object motion.

From the selected visual features and the corresponding interaction matrix, the behavior of the system will have particular properties as for stability, robustness with respect to noise or to calibration errors, robot 3D trajectory, etc. Usually, the interaction matrix is composed of highly non linear terms and does not present any decoupling properties. This is generally the case when $\mathbf{s}$ is directly chosen as $\mathbf{x}$. In some cases, it may lead to inadequate robot trajectories or even motions impossible to realize, local minimum, tasks singularities, etc. It is thus extremely important to design adequate visual features for each robot task or application, the ideal case (very difficult to obtain) being when the corresponding interaction matrix is constant, leading to a simple linear control system. To conclude in a few words, **visual servoing is basically a non linear control problem. Our Holy Grail quest is to transform it into a linear control problem.**

Furthermore, embedding visual servoing in the task function approach allows solving efficiently the redundancy problems that appear when the visual task does not constrain all the degrees of freedom of the system. It is then possible to realize simultaneously the visual task and secondary tasks such as visual inspection, or joint limits or singularities avoidance. This formalism can also be used for tasks sequencing purposes in order to deal with high level complex applications.

3.2. Visual tracking

Elaboration of object tracking algorithms in image sequences is an important issue for researches and applications related to visual servoing and more generally for robot vision. A robust extraction and real time spatio-temporal tracking process of visual cues is indeed one of the keys to success of a visual servoing task. If fiducial markers may still be useful to validate theoretical aspects in modeling and control, natural scenes with non-cooperative objects and subject to various illumination conditions have to be considered for addressing large scale realistic applications.

Most of the available tracking methods can be divided into two main classes: feature-based and model-based. The former approach focuses on tracking 2D features such as geometrical primitives (points, segments, circles,...), object contours, regions of interest, etc. The latter explicitly uses a model of the tracked objects. This can be either a 3D model or a 2D template of the object. This second class of methods usually provides a more robust solution. Indeed, the main advantage of the model-based methods is that the knowledge about the scene allows improving tracking robustness and performance, by being able to predict hidden movements of the object, detect partial occlusions and acts to reduce the effects of outliers. The challenge is to build algorithms that are fast and robust enough to meet our application requirements. Therefore, even if we still consider 2D feature tracking in some cases, our researches mainly focus on real-time 3D model-based tracking, since these approaches are very accurate, robust, and well adapted to any class of visual servoing schemes. Furthermore, they also meet the requirements of other classes of application, such as augmented reality.

3.3. Slam

Most of the applications involving mobile robotic systems (ground vehicles, aerial robots, automated submarines,...) require a reliable localization of the robot in its environment. A challenging problem is when neither the robot localization nor the map is known. Localization and mapping must then be considered concurrently. This problem is known as Simultaneous Localization And Mapping (Slam). In this case, the robot moves from an unknown location in an unknown environment and proceeds to incrementally build up a navigation map of the environment, while simultaneously using this map to update its estimated position.

Nevertheless, solving the Slam problem is not sufficient for guaranteeing an autonomous and safe navigation. The choice of the representation of the map is, of course, essential. The representation has to support the different levels of the navigation process: motion planning, motion execution and collision avoidance and, at the global level, the definition of an optimal strategy of displacement. The original formulation of the Slam problem is purely metric (since it basically consists in estimating the Cartesian situations of the robot and a set of landmarks), and it does not involve complex representations of the environment. However, it is now well recognized that **several complementary representations are needed to perform exploration, navigation, mapping, and control tasks successfully. We propose to use composite models of the environment that**

mix topological, metric, and grid-based representations. Each type of representation is well adapted to a particular aspect of autonomous navigation [7]: the metric model allows one to locate the robot precisely and plan Cartesian paths, the topological model captures the accessibility of different sites in the environment and allows a coarse localization, and finally the grid representation is useful to characterize the free space and design potential functions used for reactive obstacle avoidance. However, ensuring the consistency of these various representations during the robot exploration, and merging observations acquired from different viewpoints by several cooperative robots, are difficult problems. This is particularly true when different sensing modalities are involved. New studies to derive efficient algorithms for manipulating the hybrid representations (merging, updating, filtering...) while preserving their consistency are needed.

3.4. Scene modeling and understanding

Long-term mapping has received an increasing amount of attention during last years, largely motivated by the growing need to integrate robots into the real world wherein dynamic objects constantly change the appearance of the scene. A mobile robot evolving in such a dynamic world should not only be able to build a map of the observed environment at a specific moment, but also to maintain this map consistent over a long period of time. It has to deal with dynamic changes that can cause the navigation process to fail. However updating the map is particularly challenging in large-scale environments. To identify changes, robots have to keep a memory of the previous states of the environment and the more dynamic it is, the higher will be the number of states to manage and the more computationally intensive will be the updating process. Mapping large-scale dynamic environments is then particularly difficult as the map size can be arbitrary large. Additionally, mapping many times the whole environment is not always possible or convenient and it is useful to take advantages of methods using only a small number of observations.

A recent trend in robotic mapping is to augment low-level maps with semantic interpretation of their content, which allows to improve the robot's environmental awareness through the use of high-level concepts. In mobile robot navigation, the so-called semantic maps have already been used to improve path planning methods, mainly by providing the robot with the ability to deal with human-understandable targets.

LARSEN Team

3. Research Program

3.1. Lifelong Autonomy

3.1.1. Scientific Context

So far, only a few autonomous robots have been deployed for a long time (weeks, months, or years) outside of factories and laboratories. They are mostly mobile robots that simply “move around” (e.g., vacuum cleaners or museum “guides”) and data collecting robots (e.g., boats or underwater “gliders” that collect data about the water of the ocean).

A large part of the long-term autonomy community is focused on simultaneous localization and mapping (SLAM), with a recent emphasis on changing and outdoor environments [39], [50]. A more recent theme is life-long learning: during long-term deployment, we cannot hope to equip robots with everything they need to know, therefore some things will have to be learned along the way. Most of the work on this topic leverages machine learning and/or evolutionary algorithms to improve the ability of robots to react to unforeseen changes [39], [48].

3.1.2. Main Challenges

The first major challenge is to endow robots with a stable situation awareness in open and dynamic environments. This covers both the state estimation of the robot itself as well as the perception/representation of the environment. Both problems have been claimed to be solved but it is only the case for static environments [47].

In the LARSEN team, we aim at deployment in environments shared with humans which imply dynamic objects that degrade both the mapping and localization of a robot, especially in cluttered spaces. Moreover, when robots stay longer in the environment than for the acquisition of a snapshot map, they have to face structural changes, such as the displacement of a piece of furniture or the opening or closing of a door. The current approach is to simply update an implicitly static map with all observations with no attempt at distinguishing the suitable changes. For localization in not-too-cluttered or not-too-empty environments, this is generally sufficient as a significant fraction of the environment should remain stable. But for life-long autonomy, and in particular navigation, the quality of the map, and especially the knowledge of the stable parts, is primordial.

A second major obstacle to move robots outside of labs and factories is their fragility: current robots often break in a few hours, if not a few minutes. This fragility mainly stems from the overall complexity of robotic systems, which involve many actuators, many sensors, and complex decisions, and from the diversity of situations that robots can encounter. Low-cost robots exacerbate this issue because they can be broken in many ways (high-quality material is expensive), because they have low self-sensing abilities (sensors are expensive and increase the overall complexity), and because they are typically targeted towards non-controlled environments (e.g., houses rather than factories, in which robots are protected from most unexpected events). More generally, this fragility is a symptom of the lack of adaptive abilities in current robots.

3.1.3. Angle of Attack

To solve the state estimation problem, our approach is to combine classical estimation filters (Extended Kalman Filters, Unscented Kalman Filters, or particle filters) with a Bayesian reasoning model in order to internally simulate various configurations of the robot in its environment. This should allow for adaptive estimation that can be used as one aspect of long-term adaptation. To handle dynamic and structural changes in an environment, we aim at assessing, for each piece of observation, whether it is static or not.

We also plan to address active sensing to improve the situation awareness of robots. Literally, active sensing is the ability of an interacting agent to act so as to control what it senses from its environment with the typical objective of acquiring information about this environment. A formalism for representing and solving active sensing problems has already been proposed by members of the team [38] and we aim to use this to formalize decision making problems of improving situation awareness.

Situation awareness of robots can also be tackled by cooperation, whether it be between robots or between robots and sensors in the environment (led out intelligent spaces) or between robots and humans. This is in rupture with classical robotics, in which robots are conceived as self-contained. But, in order to cope with as diverse environments as possible, these classical robots use precise, expensive, and specialized sensors, whose cost prohibits their use in large-scale deployments for service or assistance applications. Furthermore, when all sensors are on the robot, they share the same point of view on the environment, which is a limit for perception. Therefore, we propose to complement a cheaper robot with sensors distributed in a target environment. This is an emerging research direction that shares some of the problematics of multi-robot operation and we are therefore collaborating with other teams at Inria that address the issue of communication and interoperability.

To address the fragility problem, the traditional approach is to first diagnose the situation, then use a planning algorithm to create/select a contingency plan. But, again, this calls for both expensive sensors on the robot for the diagnosis and extensive work to predict and plan for all the possible faults that, in an open and dynamic environment, are almost infinite. An alternative approach is then to skip the diagnosis and let the robot discover by trial and error a behavior that works in spite of the damage with a reinforcement learning algorithm [57], [48]. However, current reinforcement learning algorithms require hundreds of trials/episodes to learn a single, often simplified, task [48], which makes them impossible to use for real robots and more ambitious tasks. **We therefore need to design new trial-and-error algorithms that will allow robots to learn with a much smaller number of trials (typically, a dozen).** We think the key idea is to guide online learning on the physical robot with dynamic simulations. For instance, in our recent work, we successfully mixed evolutionary search in simulation, physical tests on the robot, and machine learning to allow a robot to recover from physical damage [49], [2].

A final approach to address fragility is to deploy several robots or a swarm of robots or to make robots evolve in an active environment. We will consider several paradigms such as (1) those inspired from collective natural phenomena in which the environment plays an active role for coordinating the activity of a huge number of biological entities such as ants and (2) those based on online learning [46]. We envision to transfer our knowledge of such phenomenon to engineer new artificial devices such as an intelligent floor (which is in fact a spatially distributed network in which each node can sense, compute and communicate with contiguous nodes and can interact with moving entities on top of it) in order to assist people and robots (see the principle in [55], [46], [37]).

3.2. Natural Interaction with Robotic Systems

3.2.1. Scientific Context

Interaction with the environment is a primordial requirement for an autonomous robot. When the environment is sensorized, the interaction can include localizing, tracking, and recognizing the behavior of robots and humans. One specific issue lies in the lack of predictive models for human behavior and a critical constraint arises from the incomplete knowledge of the environment and the other agents.

On the other hand, when working in the proximity of or directly with humans, robots must be capable of safely interacting with them, which calls upon a mixture of physical and social skills. Currently, robot operators are usually trained and specialized but potential end-users of robots for service or personal assistance are not skilled robotics experts, which means that the robot needs to be accepted as reliable, trustworthy and efficient [61]. Most Human-Robot Interaction (HRI) studies focus on verbal communication [56] but applications such as assistance robotics require a deeper knowledge of the intertwined exchange of social and physical signals to provide suitable robot controllers.

3.2.2. Main Challenges

We are here interested in building the bricks for a situated Human-Robot Interaction (HRI) addressing both the physical and social dimension of the close interaction, and the cognitive aspects related to the analysis and interpretation of human movement and activity.

The combination of physical and social signals into robot control is a crucial investigation for assistance robots [58] and robotic co-workers [53]. A major obstacle is the control of physical interaction (precisely, the control of contact forces) between the robot and the human while both partners are moving. In mobile robots, this problem is usually addressed by planning the robot movement taking into account the human as an obstacle or as a target, then delegating the execution of this "high-level" motion to whole-body controllers, where a mixture of weighted tasks is used to account for the robot balance, constraints, and desired end-effector trajectories [43].

The first challenge is to make these controllers easier to deploy in real robotics systems, as currently they require a lot of tuning and can become very complex to handle the interaction with unknown dynamical systems such as humans. Here, the key is to combine machine learning techniques with such controllers.

The second challenge is to make the robot react and adapt online to the human feedback, exploiting the whole set of measurable verbal and non-verbal signals that humans naturally produce during a physical or social interaction. Technically, this means finding the optimal policy that adapts the robot controllers online, taking into account feedback from the human. Here, we need to carefully identify the significant feedback signals or some metrics of human feedback. In real-world conditions (i.e., outside the research laboratory environment) the set of signals is technologically limited by the robot's and environmental sensors and the onboard processing capabilities.

The third challenge is for a robot to be able to identify and track people on board. The motivation is to be able to estimate online either the position, the posture, or even moods and intentions of persons surrounding the robot. The main challenge is to be able to do that online, in real-time and in cluttered environments.

3.2.3. Angle of Attack

Our key idea is to exploit the physical and social signals produced by the human during the interaction with the robot and the environment in controlled conditions, to learn simple models of human behavior and consequently to use these models to optimize the robot movements and actions. In a first phase, we will exploit human physical signals (e.g., posture and force measurements) to identify the elementary posture tasks during balance and physical interaction. The identified model will be used to optimize the robot whole-body control as prior knowledge to improve both the robot balance and the control of the interaction forces. Technically, we will combine weighted and prioritized controllers with stochastic optimization techniques. To adapt online the control of physical interaction and make it possible with human partners that are not robotics experts, we will exploit verbal and non-verbal signals (e.g., gaze, touch, prosody). The idea here is to estimate online from these signals the human intent along with some inter-individual factors that the robot can exploit to adapt its behavior, maximizing the engagement and acceptability during the interaction.

Another promising approach already investigated in the LARSEN team is the capability for a robot and/or an intelligent space to localize humans in its surrounding environment and to understand their activities. This is an important issue to handle both for safe and efficient human-robot interaction.

Simultaneous Tracking and Activity Recognition (STAR) [60] is an approch we want to develop. The activity of a person is highly correlated with his position, and this approach aims at combining tracking and activity recognition to benefit one from another. By tracking the individual, the system may help infer its possible activity, while by estimating the activity of the individual, the system may make a better prediction of his possible future positions (which can be very effective in case of occlusion). This direction has been tested with simulator and particle filters [45], and one promising direction would be to couple STAR with decision making formalisms like partially observable Markov decision processes, POMDPs). This would allow to formalize problems such as deciding which action to take given an estimate of the human location and activity. This could also formalize other problems linked to the active sensing direction of the team: how the robotic system might choose its actions in order to have a better estimate of the human location and activity (for instance by moving in the environment or by changing the orientation of its cameras)?

Another issue we want to address is robotic human body pose estimation. Human body pose estimation consists of tracking body parts by analyzing a sequence of input images from single or multiple cameras.

Human posture analysis is of high value for human robot interaction and activity recognition. However, even if the arrival of new sensors like RGB-D cameras has simplified the problem, it still poses a great challenge, especially if we want to do it online, on a robot and in realistic world conditions (cluttered environment). This is even more difficult for a robot to bring together different capabilities both at the perception and navigation level [44]. This will be tackled through different techniques, going from Bayesian state estimation (particle filtering), to learning, active and distributed sensing.

LINKMEDIA Project-Team

3. Research Program

3.1. Scientific background

LINKMEDIA is a multidisciplinary research team, with multimedia data as the main object of study. We are guided by the data and their specificity—semantically interpretable, heterogeneous and multimodal, available in large amounts, unstructured and disconnected—, as well as by the related problems and applications.

With multimedia data at the center, orienting our choices of methods and algorithms and serving as a basis for experimental validation, the team is directly contributing to the following scientific fields:

- multimedia: content-based analysis; multimodal processing and fusion; multimedia applications;
- computer vision: compact description of images; object and event detection;
- natural language processing: topic segmentation; information extraction;
- information retrieval: high-dimensional indexing; approximate k-nn search; efficient set comparison.

LINKMEDIA also takes advantage of advances in the following fields, adapting recent developments to the multimedia area:

- signal processing: image processing; compression;
- machine learning: deep architectures; structured learning; adversarial learning;
- security: data encryption; differential privacy;
- data mining: time series mining and alignment; pattern discovery; knowledge extraction.

3.2. Workplan

Research activities in LINKMEDIA are organized along three major lines of research which build upon the scientific domains already mentioned.

3.2.1. Unsupervised motif discovery

As an alternative to supervised learning techniques, unsupervised approaches have emerged recently in multimedia with the goal of discovering directly patterns and events of interest from the data, in a totally unsupervised manner. In the absence of prior knowledge on what we are interested in, meaningfulness can be judged based on one of three main criteria: unexpectedness, saliency and recurrence. This last case posits that repeating patterns, known as motifs, are potentially meaningful, leading to recent work on the unsupervised discovery of motifs in multimedia data [54], [52], [53].

LINKMEDIA seeks to *develop unsupervised motif discovery approaches which are both accurate and scalable*. In particular, we consider the discovery of repeating objects in image collections and the discovery of repeated sequences in video and audio streams. Research activities are organized along the following lines:

- developing the scientific basis for scalable motif discovery: sparse histogram representations; efficient co-occurrence counting; geometry and time aware indexing schemes;
- designing and evaluating accurate and scalable motif discovery algorithms applied to a variety of multimedia content: exploiting efficient geometry or time aware matching functions; fast approximate dynamic time warping; symbolic representations of multimedia data, in conjunction with existing symbolic data mining approaches;
- developing methodology for the interpretation, exploitation and evaluation of motif discovery algorithms in various use-cases: image classification; video stream monitoring; transcript-free natural language processing (NLP) for spoken document.

3.2.2. Description and structuring

Content-based analysis has received a lot of attention from the early days of multimedia, with an extensive use of supervised machine learning for all modalities [56], [48]. Progress in large scale entity and event recognition in multimedia content has made available general purpose approaches able to learn from very large data sets and performing fairly decently in a large number of cases. Current solutions are however limited to simple, homogeneous, information and can hardly handle structured information such as hierarchical descriptions, tree-structured or nested concepts.

LINKMEDIA aims at *expanding techniques for multimedia content modeling, event detection and structure analysis*. The main transverse research lines that LINKMEDIA will develop are as follows:

- context-aware content description targeting (homogeneous) collections of multimedia data: latent variable discovery; deep feature learning; motif discovery;
- secure description to enable privacy and security aware multimedia content processing: leveraging encryption and obfuscation; exploring adversarial machine learning in a multimedia context; privacy-oriented image processing;
- multilevel modeling with a focus on probabilistic modeling of structured multimodal data: multiple kernels; structured machine learning; conditional random fields.

3.2.3. Linking and collection data model

Creating explicit links between media content items has been considered on different occasions, with the goal of seeking and discovering information by browsing, as opposed to information retrieval via ranked lists of relevant documents. Content-based link creation has been initially addressed in the hypertext community for well-structured texts [47] and was recently extended to multimedia content [57], [51], [50]. The problem of organizing collections with links remains mainly unsolved for large heterogeneous collections of unstructured documents, with many issues deserving attention: linking at a fine semantic grain; selecting relevant links; characterizing links; evaluating links; etc.

LINKMEDIA targets pioneering research on media linking by *developing scientific ground, methodology and technology for content-based media linking* directed to applications exploiting rich linked content such as navigation or recommendation. Contributions are concentrated along the following lines:

- algorithmic of linked media for content-based link authoring in multimedia collections: time-aware graph construction; multimodal hypergraphs; large scale k-nn graphs;
- link interpretation and characterization to provide links semantics for interpretability: text alignment; entity linking; intention vs. extension;
- linked media usage and evaluation: information retrieval; summarization; data models for navigation; link prediction.

LINKS Project-Team

3. Research Program

3.1. Background

The main objective of LINKS is to develop methods for querying and managing linked data collections. Even though open linked data is the most prominent example, we will focus on hybrid linked data collections, which are collections of semi-structured datasets in hybrid formats: graph-based, RDF, relational, and NOSQL. The elements of these datasets may be linked, either by pointers or by additional relations between the elements of the different datasets, for instance the “same-as” or “member-of” relations as in RDF.

The advantage of traditional data models is that there exist powerful querying methods and technologies that one might want to preserve. In particular, they come with powerful schemas that constraint the possible manners in which knowledge is represented to a finite number of patterns. The exhaustiveness of these patterns is essential for writing of queries that cover all possible cases. Pattern violations are excluded by schema validation. In contrast, RDF schema languages such as RDFS can only enrich the relations of a dataset by new relations, which also helps for query writing, but which cannot constraint the number of possible patterns, so that they do not come with any reasonable notion of schema validation.

The main weakness of traditional formats, however, is that they do not scale to large data collections as stored on the Web, while the RDF data models scales well to very big collections such as linked open data. Therefore, our objective is to study mixed data collections, some of which may be in RDF format, in which we can lift the advantages of smaller datasets in traditional formats to much larger linked data collections. Such data collections are typically distributed over the internet, that some data sources have rigid query facilities that cannot be easily adapted or extended.

The main assumption that we impose in order to enable the logical approach, is that the given linked data collection must be correct in most dimensions. This means that all datasets are well-formed with respect to their available constraints and schemas, and clean with respect to the data values in most of the components of the relations in the datasets. One of the challenges is to integrate good quality RDF datasets into this setting, another is to clean the incorrect data in those dimensions that are less proper. It remains to be investigated in how far these assumptions can be maintained in realistic applications, and how much they can be weakened otherwise.

For querying linked data collections, the main problems are to resolve the heterogeneity of data formats and schemas, to understand the efficiency and expressiveness of recursive queries, that can follow links repeatedly, to answer queries under constraints, and to optimize query answering algorithms based on static analysis. When linked data is dynamically created, exchanged, or updated, the problems are how to process linked data incrementally, and how to manage linked data collections that change dynamically. In any case (static and dynamic) one needs to find appropriate schema mappings for linking semi-structured datasets. We will study how to automatize parts of this search process by developing symbolic machine learning techniques for linked data collections.

3.2. Querying Heterogeneous Linked Data

Our main objective is to query collections of linked datasets. In the static setting, we consider two kinds of links: explicit links between elements of the datasets, such as equalities or pointers, and logical links between relations of different datasets such as schema mappings. In the dynamic setting, we permit a third kind of links that point to “intentional” relations computable from a description, such as the application of a Web service or the application of a schema mapping.

We believe that collections of linked datasets are usually too big to ensure a global knowledge of all datasets. Therefore, schema mappings and constraints should remain between pairs of datasets. Our main goal is to be able to pose a query on a collection of datasets, while accounting for the possible recursive effects of schema mappings. For illustration, consider a ring of datasets D_1, D_2, D_3 linked by schema mappings M_1, M_2, M_3 that tell us how to complete a database D_i by new elements from the next database in the cycle.

The mappings M_i induce three intentional datasets I_1, I_2, and I_3, such that I_i contains all elements from D_i and all elements implied by M_i from the next intentional dataset in the ring:

$$I_1 = D_1 \cup M_1(I_2), \quad I_2 = D_2 \cup M_2(I_3), \quad I_3 = D_3 \cup M_3(I_1)$$

Clearly, the global information collected by the intentional datasets depends recursively on all three original datasets D_i. Queries to the global information can now be specified as standard queries to the intentional databases I_i. However, we will never materialize the intentional databases I_i. Instead, we can rewrite queries on one of the intentional datasets I_i to recursive queries on the union of the original datasets D_1, D_2, and D_3 with their links and relations. Therefore, a query answering algorithm is needed for recursive queries, that chases the "links" between the D_i in order to compute the part of I_i needed for the purpose of query answering.

This illustrates that we must account for the graph data models when dealing with linked data collections whose elements are linked, and that query languages for such graphs must provide recursion in order to chase links. Therefore, we will have to study graph databases with recursive queries, such as RDF graphs with SPARQL queries, but also other classes of graph databases and queries.

We study schemas and mappings between datasets with different kinds of data models and the complexity of evaluating recursive queries over graphs. In order to use schema mapping for efficiently querying the different datasets, we need to optimize the queries by taking into account the mappings. Therefore, we will study static analysis of schema mappings and recursive queries. Finally, we develop concrete applications in which our fundamental techniques can be applied.

3.3. Managing Dynamic Linked Data

With the quick growth of the information technology on the Web, more and more Web data gets created dynamically every day, for instance by smartphones, industrial machines, users of social networks, and all kinds of sensors. Therefore, large amounts of dynamic data need to be exchanged and managed by various data-centric web services, such as online shops, online newspapers, and social networks.

Dynamic data is often created by the application of some kind of service on the Web. This kind of data is intentional in the same spirit as the intentional data specified by the application of a schema mapping, or the application of some query to the hidden Web. Therefore, we will consider a third kind of links in the dynamic setting, that map to intentional data specified by whatever kind of function application. Such a function can be defined in data-centric programming languages, in the style of Active XML, XSLT, and NoSQL languages.

The dynamicity of data adds a further dimension to the challenges for linked data collections that we described before, while all the difficulties remain valid. One of the new aspects is that intentional data may be produced incrementally, as for instance when exchanged over data streams. Therefore, one needs incremental algorithms able to evaluate queries on incomplete linked data collections, that are extended or updated incrementally. Note that incremental data may be produced without end, such as a Twitter stream, so that one cannot wait for its completion. Instead, one needs to query and manage dynamic data with as low latency as possible. Furthermore, all static analysis problems are to be re-investigated in the presence of dynamic data.

Another aspect of dynamic data is distribution over the Web, and thus parallel processing as in the cloud. This raises the typical problems coming with data distribution: huge data sources cannot be moved without very high costs, while data must be replicated for providing efficient parallel access. This makes it difficult, if not impossible, to update replicated data consistently. Therefore, the consistency assumption has been removed by NoSQL databases for instance, while parallel algorithmic is limited to naive parallelisation (i.e. map/reduce) where only few data needs to be exchanged.

We will investigate incremental query evaluation for distributed data-centered programming languages for linked data collections, dynamic updates as needed for linked data management, and static analysis for linked data workflows.

3.4. Linking Graphs

When datasets from independent sources are not linked with existing schema mappings, we would like to investigate symbolic machine learning solutions for inferring such mappings in order to define meaningful links between data from separate sources. This problem can be studied for various kinds of linked data collections. Before presenting the precise objectives, we will illustrate our approach on the example of linking data in two independent graphs: an address book of a research institute containing detailed personnel information and a (global) bibliographic database containing information on papers and their authors.

We remind that a schema allows to identify a collection of types each grouping objects from the same semantic class e.g., the collection of all persons in the address book and the collection of all authors in the bibliography database. As a schema is often lacking or underspecified in graph data models, we intend to investigate inference methods based on structural similarity of graph fragments used to describe objects from the same class in a given document e.g., in the bibliographic database every author has a name and a number of affiliations, while a paper has a title and a number of authors. Furthermore, our inference methods will attempt to identify, for every type, a set of possible keys, where by key we understand a collection of attributes of an object that uniquely identifies such an object in its semantic class. For instance, for a person in the address book two examples of a key are the name of the person and the office phone number of that person.

In the next step, we plan to investigate employing existing entity linkage solutions to identify pairs of types from different databases whose instances should be linked using compatible keys. For instance, persons in the address book should be linked with authors in the bibliographical database using the name as the compatible key. Linking the same objects (represented in different ways) in two databases can be viewed as an instance of a mapping between the two databases. Such mapping is, however, discriminatory because it typically maps objects from a specific subset of objects of given types. For instance, the mapping implied by linking persons in the address book with authors in the bibliographic database involves in fact researchers, a subgroup of personnel of the research institute, and authors affiliated with the research institute. Naturally, a subset of objects of a given type, or a subtype, can be viewed as a result of a query on the set of all objects, which on very basic level illustrates how learning data mappings can be reduced to learning queries.

While basic mappings link objects of the same type, more general mappings define how the same type of information is represented in two different databases. For instance, the email address and the postal address of an individual may be represented in one way in the address book and in another way in the bibliographic databases, and naturally, the query asking for the email address and the postal address of a person identified by a given name will differ from one database to the other. While queries used in the context of linking objects of compatible types are essentially unary, queries used in the context of linking information are n-ary and we plan to approach inference of general database mappings by investigating and employing algorithms for inference of n-ary queries.

An important goal in this research is elaborating a formal definition of *learnability* (feasibility of inference) of a given class of concepts (schemas of queries). We plan to following the example of Gold (1967), which requires not only the existence of an efficient algorithm that infers concepts consistent with the given input but the ability to infer every concept from the given class with a sufficiently informative input. Naturally, learnability depends on two parameters. The first parameter is the class of concepts i.e., a class of schema and a class of queries, from which the goal concept is to be inferred. The second parameter is the type of input that an inference algorithm is given. This can be a set of examples of a concept e.g., instances of RDF databases for which we wish to construct a schema or a selection of nodes that a goal query is to select. Alternatively, a more general interactive scenario can be used where the learning algorithm inquires the user about the goal concept e.g., by asking to indicate whether a given node is to be selected or not (as membership queries of Angluin (1987)). In general, the richer the input is, the richer class of concepts can be handled, however, the richer class of queries is to be handled, the higher computational cost is to be expected. The primary task is to find a good compromise and identify classes of concepts that are of high practical value, allow efficient inference with possibly simple type of input.

The main open problem for graph-shaped data studied by Links are how to infer queries, schemas, and schema-mappings for graph-structured data.

MAGNET Project-Team

3. Research Program

3.1. Introduction

The main objective of MAGNET is to develop original machine learning methods for networked data in order to build applications like browsing, monitoring and recommender systems, and more broadly information extraction in information networks. We consider information networks in which the data consist of both feature vectors and texts. We model such networks as (multiple) (hyper)graphs wherein nodes correspond to entities (documents, spans of text, users, ...) and edges correspond to relations between entities (similarity, answer, co-authoring, friendship, ...). Our main research goal is to propose new on-line and batch learning algorithms for various problems (node classification / clustering, link classification / prediction) which exploit the relationships between data entities and, overall, the graph topology. We are also interested in searching for the best hidden graph structure to be generated for solving a given learning task. Our research will be based on generative models for graphs, on machine learning for graphs and on machine learning for texts. The challenges are the dimensionality of the input space, possibly the dimensionality of the output space, the high level of dependencies between the data, the inherent ambiguity of textual data and the limited amount of human labeling. An additional challenge will be to design scalable methods for large information networks. Hence, we will explore how sampling, randomization and active learning can be leveraged to improve the scalability of the proposed algorithms.

Our research program is organized according to the following questions:

1. How to go beyond vectorial classification models in Natural Language Processing (NLP) tasks?
2. How to adaptively build graphs with respect to the given tasks? How to create networks from observations of information diffusion processes?
3. How to design methods able to achieve a good trade-off between predictive accuracy and computational complexity?
4. How to go beyond strict node homophilic/similarity assumptions in graph-based learning methods?

3.2. Beyond Vectorial Models for NLP

One of our overall research objectives is to derive graph-based machine learning algorithms for natural language and text information extraction tasks. This section discusses the motivations behind the use of graph-based ML approaches for these tasks, the main challenges associated with it, as well as some concrete projects. Some of the challenges go beyond NLP problems and will be further developed in the next sections. An interesting aspect of the project is that we anticipate some important cross-fertilizations between NLP and ML graph-based techniques, with NLP not only benefiting from but also pushing ML graph-based approaches into new directions.

Motivations for resorting to graph-based algorithms for texts are at least threefold. First, online texts are organized in networks. With the advent of the web, and the development of forums, blogs, and micro-blogging, and other forms of social media, text productions have become strongly connected. Interestingly, NLP research has been rather slow in coming to terms with this situation, and most of the literature still focus on document-based or sentence-based predictions (wherein inter-document or inter-sentence structure is not exploited). Furthermore, several multi-document tasks exist in NLP (such as multi-document summarization and cross-document coreference resolution), but most existing work typically ignore document boundaries and simply apply a document-based approach, therefore failing to take advantage of the multi-document dimension [40], [43].

A second motivation comes from the fact that most (if not all) NLP problems can be naturally conceived as graph problems. Thus, NLP tasks often involve discovering a relational structure over a set of text spans (words, phrases, clauses, sentences, etc.). Furthermore, the *input* of numerous NLP tasks is also a graph; indeed, most end-to-end NLP systems are conceived as pipelines wherein the output of one processor is in the input of the next. For instance, several tasks take POS tagged sequences or dependency trees as input. But this structured input is often converted to a vectorial form, which inevitably involves a loss of information.

Finally, graph-based representations and learning methods appear to address some core problems faced by NLP, such as the fact that textual data are typically not independent and identically distributed, they often live on a manifold, they involve very high dimensionality, and their annotations is costly and scarce. As such, graph-based methods represent an interesting alternative to, or at least complement, structured prediction methods (such as CRFs or structured SVMs) commonly used within NLP. Graph-based methods, like label propagation, have also been shown to be very effective in semi-supervised settings, and have already given some positive results on a few NLP tasks [22], [45].

Given the above motivations, our first line of research will be to investigate how one can leverage an underlying network structure (e.g., hyperlinks, user links) between documents, or text spans in general, to enhance prediction performance for several NLP tasks. We think that a “network effect”, similar to the one that took place in Information Retrieval (with the Page Rank algorithm), could also positively impact NLP research. A few recent papers have already opened the way, for instance in attempting to exploit Twitter follower graph to improve sentiment classification [44].

Part of the challenge here will be to investigate how adequately and efficiently one can model these problems as instances of more general graph-based problems, such as node clustering/classification or link prediction discussed in the next sections. In a few cases, like text classification or sentiment analysis, graph modeling appears to be straightforward: nodes correspond to texts (and potentially users), and edges are given by relationships like hyperlinks, co-authorship, friendship, or thread membership. Unfortunately, modeling NLP problems as networks is not always that obvious. From the one hand, the right level of representation will probably vary depending on the task at hand: the nodes will be sentences, phrases, words, etc. From the other hand, the underlying graph will typically not be given a priori, which in turn raises the question of how we construct it. A preliminary discussion of the issue of optimal graph construction for semi-supervised learning in NLP is given in [22], [48]. We identify the issue of adaptive graph construction as an important scientific challenge for machine learning on graphs in general, and we will discuss it further in Section 3.3 .

As noted above, many NLP tasks have been recast as structured prediction problems, allowing to capture (some of the) output dependencies. How to best combine structured output and graph-based ML approaches is another challenge that we intend to address. We will initially investigate this question within a semi-supervised context, concentrating on graph regularization and graph propagation methods. Within such approaches, labels are typically binary or in a small finite set. Our objective is to explore how one propagates an exponential number of *structured labels* (like a sequence of tags or a dependency tree) through graphs. Recent attempts at blending structured output models with graph-based models are investigated in [45], [33]. Another related question that we will address in this context is how does one learn with *partial labels* (like partially specified tag sequence or tree) and use the graph structure to complete the output structure. This last question is very relevant to NLP problems where human annotations are costly; being able to learn from partial annotations could therefore allow for more targeted annotations and in turn reduced costs [35].

The NLP tasks we will mostly focus on are coreference resolution and entity linking, temporal structure prediction, and discourse parsing. These tasks will be envisioned in both document and cross-document settings, although we expect to exploit inter-document links either way. Choices for these particular tasks is guided by the fact that they are still open problems for the NLP community, they potentially have a high impact for industrial applications (like information retrieval, question answering, etc.), and we already have some expertise on these tasks in the team (see for instance [34], [30], [32]). As a midterm goal, we also plan to work on tasks more directly relating to micro-blogging, such sentiment analysis and the automatic thread structuring of technical forums; the latter task is in fact an instance of rhetorical structure prediction [47].

We have already initiated some work on the coreference resolution with graph-based learning, by casting the problem as an instance of spectral clustering [32].

3.3. Adaptive Graph Construction

In most applications, edge weights are computed through a complex data modeling process and convey crucially important information for classifying nodes, making it possible to infer information related to each data sample even exploiting the graph topology solely. In fact, a widespread approach to several classification problems is to represent the data through an undirected weighted graph in which edge weights quantify the similarity between data points. This technique for coding input data has been applied to several domains, including classification of genomic data [42], face recognition [31], and text categorization [36].

In some cases, the full adjacency matrix is generated by employing suitable similarity functions chosen through a deep understanding of the problem structure. For example for the TF-IDF representation of documents, the affinity between pairs of samples is often estimated through the cosine measure or the χ^2 distance. After the generation of the full adjacency matrix, the second phase for obtaining the final graph consists in an edge sparsification/reweighting operation. Some of the edges of the clique obtained in the first step are pruned and the remaining ones can be reweighted to meet the specific requirements of the given classification problem. Constructing a graph with these methods obviously entails various kinds of loss of information. However, in problems like node classification, the use of graphs generated from several datasets can lead to an improvement in accuracy ([49], [23], [24]). Hence, the transformation of a dataset into a graph may, at least in some cases, partially remove various kinds of irregularities present in the original datasets, while keeping some of the most useful information for classifying the data samples. Moreover, it is often possible to accomplish classification tasks on the obtained graph using a running time remarkably lower than is needed by algorithms exploiting the initial datasets, and a suitable sparse graph representation can be seen as a compressed version of the original data. This holds even when input data are provided in a online/stream fashion, so that the resulting graph evolves over time.

In this project we will address the problem of adaptive graph construction towards several directions. The first one is about how to choose the best similarity measure given the objective learning task. This question is related to the question of metric and similarity learning ([25], [26]) which has not been considered in the context of graph-based learning. In the context of structured prediction, we will develop approaches where output structures are organized in graphs whose similarity is given by top-k outcomes of greedy algorithms.

A different way we envision adaptive graph construction is in the context of semi-supervised learning. Partial supervision can take various forms and an interesting and original setting is governed by two currently studied applications: detection of brain anomaly from connectome data and polls recommendation in marketing. Indeed, for these two applications, a partial knowledge of the information diffusion process can be observed while the network is unknown or only partially known. An objective is to construct (or complete) the network structure from some local diffusion information. The problem can be formalized as a graph construction problem from partially observed diffusion processes. It has been studied very recently in [38]. In our case, the originality comes either from the existence of different sources of observations or from the large impact of node contents in the network.

We will study how to combine graphs defined by networked data and graphs built from flat data to solve a given task. This is of major importance for information networks because, as said above, we will have to deal with multiple relations between entities (texts, spans of texts, ...) and also use textual data and vectorial data.

3.4. Prediction on Graphs and Scalability

As stated in the previous sections, graphs as complex objects provide a rich representation of data. Often enough the data is only partially available and the graph representation is very helpful in predicting the unobserved elements. We are interested in problems where the complete structure of the graph needs to be recovered and only a fraction of the links is observed. The link prediction problem falls into this category. We are also interested in the recommendation and link classification problems which can be seen as graphs where the structure is complete but some labels on the links (weights or signs) are missing. Finally we are also interested in labeling the nodes of the graph, with class or cluster memberships or with a real value, provided that we have (some information about) the labels for some of the nodes.

The semi-supervised framework will be also considered. A midterm research plan is to study how graph regularization models help for structured prediction problems. This question will be studied in the context of NLP tasks, as noted in Section 3.2 , but we also plan to develop original machine learning algorithms that have a more general applicability. Inputs are networks whose nodes (texts) have to be labeled by structures. We assume that structures lie in some manifold and we want to study how labels can propagate in the network. One approach is to find a smooth labeling function corresponding to an harmonic function on both manifolds in input and output.

Scalability is one of the main issues in the design of new prediction algorithms working on networked data. It has gained more and more importance in recent years, because of the growing size of the most popular networked data that are now used by millions of people. In such contexts, learning algorithms whose computational complexity scales quadratically, or slower, in the number of considered data objects (usually nodes or edges, depending on the task) should be considered impractical.

These observations lead to the idea of using graph sparsification techniques in order to work on a part of the original network for getting results that can be easily extended and used for the whole original input. A sparsified version of the original graph can often be seen as a subset of the initial input, i.e. a suitably selected input subgraph which forms the training set (or, more in general, it is included in the training set). This holds even for the active setting. A simple example could be to find a spanning tree of the input graph, possibly using randomization techniques, with properties such that we are allowed to obtain interesting results for the initial graph dataset. We have started to explore this research direction for instance in [46].

At the level of mathematical foundations, the key issue to be addressed in the study of (large-scale) random networks also concerns the segmentation of network data into sets of independent and identically distributed observations. If we identify the data sample with the whole network, as it has been done in previous approaches [37], we typically end up with a set of observations (such as nodes or edges) which are highly interdependent and hence overly violate the classic i.i.d. assumption. In this case, the data scale can be so large and the range of correlations can be so wide, that the cost of taking into account the whole data and their dependencies is typically prohibitive. On the contrary, if we focus instead on a set of subgraphs independently drawn from a (virtually infinite) target network, we come up with a set of independent and identically distributed observations—namely the subgraphs themselves, where subgraph sampling is the underlying ergodic process [28]. Such an approach is one principled direction for giving novel statistical foundations to random network modeling. At the same time, because one shifts the focus from the whole network to a set of subgraphs, complexity issues can be restricted to the number of subgraphs and their size. The latter quantities can be controlled much more easily than the overall network size and dependence relationships, thus allowing to tackle scalability challenges through a radically redesigned approach.

Another way to tackle scalability problems is to exploit the inherent decentralized nature of very large graphs. Indeed, in many situations very large graphs are the abstract view of the digital activities of a very large set of users equipped with their own device. Nowadays, smartphones, tablets and even sensors have storage and computation power and gather a lot of data that serve to analytics, prediction, suggestion and personalized recommendation. Gathering all user data in large data centers is costly because it requires oversized infrastructures with huge energy consumption and large bandwith networks. Even though cloud architectures can optimize such infrastructures, data concentration is also prone to security leaks, lost of privacy and data governance for end users. The alternative we have started to develop in Magnet is to devise decentralized, private and personalized machine learning algorithms so that they can be deployed in the personal devices. The key challenges are therefore to learn in a collaborative way in a network of learners and to preserve privacy and control on personal data.

3.5. Beyond Homophilic Relationships

In many cases, algorithms for solving node classification problems are driven by the following assumption: linked entities tend to be assigned to the same class. This assumption, in the context of social networks, is known as homophily ([29], [39]) and involves ties of every type, including friendship, work, marriage, age, gender, and so on. In social networks, homophily naturally implies that a set of individuals can be parted into subpopulations that are more cohesive. In fact, the presence of homogeneous groups sharing common interests is a key reason for affinity among interconnected individuals, which suggests that, in spite of its simplicity, this principle turns out to be very powerful for node classification problems in general networks.

Recently, however, researchers have started to consider networked data where connections may also carry a negative meaning. For instance, disapproval or distrust in social networks, negative endorsements on the Web. Although the introduction of signs on graph edges appears like a small change from standard weighted graphs, the resulting mathematical model, called signed graphs, has an unexpectedly rich additional complexity. For example, their spectral properties, which essentially all sophisticated node classification algorithms rely on, are different and less known than those of graphs. Signed graphs naturally lead to a specific inference problem that we have discussed in previous sections: link classification. This is the problem of predicting signs of links in a given graph. In online social networks, this may be viewed as a form of sentiment analysis, since we would like to semantically categorize the relationships between individuals.

Another way to go beyond homophily between entities will be studied using our recent model of hypergraphs with bipartite hyperedges [41]. A bipartite hyperedge connects two ends which are disjoint subsets of nodes. Bipartite hyperedges is a way to relate two collections of (possibly heterogeneous) entities represented by nodes. In the NLP setting, while hyperedges can be used to model bags of words, bipartite hyperedges are associated with relationships between bags of words. But each end of bipartite hyperedges is also a way to represent complex entities, gathering several attribute values (nodes) into hyperedges viewed as records. Our hypergraph notion naturally extends directed and undirected weighted graph. We have defined a spectral theory for this new class of hypergraphs and opened a way to smooth labeling on sets of nodes. The weighting scheme allows to weigh the participation of each node to the relationship modeled by bipartite hyperedges accordingly to an equilibrium condition. This condition provides a competition between nodes in hyperedges and allows interesting modeling properties that go beyond homophily and similarity over nodes (the theoretical analysis of our hypergraphs exhibits tight relationships with signed graphs). Following this competition idea, bipartite hyperedges are like matches between two teams and examples of applications are team creation. The basic tasks we are interested in are hyperedge classification, hyperedge prediction, node weight prediction. Finally, hypergraphs also represent a way to summarize or compress large graphs in which there exists highly connected couples of (large) subsets of nodes.

MAGRIT Project-Team

3. Research Program

3.1. Matching and 3D tracking

One of the most basic problems currently limiting AR applications is the registration problem. The objects in the real and virtual worlds must be properly aligned with respect to each other, or the illusion that the two worlds coexist will be compromised.

As a large number of potential AR applications are interactive, real time pose computation is required. Although the registration problem has received a lot of attention in the computer vision community, the problem of real-time registration is still far from being a solved problem, especially for unstructured environments. Ideally, an AR system should work in all environments, without the need to prepare the scene ahead of time, independently of the variations in experimental conditions (lighting, weather condition,...) which may exist between the application and the time the model of the scene was acquired.

For several years, the MAGRIT project has been aiming at developing on-line and marker-less methods for camera pose computation. The main difficulty with on-line tracking is to ensure robustness of the process over time. For off-line processes, robustness is achieved by using spatial and temporal coherence of the considered sequence through move-matching techniques. To get robustness for open-loop systems, we have investigated various methods, ranging from statistical methods to the use of hybrid camera/sensor systems. Many of these methods are dedicated to piecewise-planar scenes and combine the advantage of move-matching methods and model-based methods. In order to reduce statistical fluctuations in viewpoint computation, which lead to unpleasant jittering or sliding effects, we have also developed model selection techniques which allow us to noticeably improve the visual impression and to reduce drift over time. Another line of research which has been considered in the team to improve the reliability and the robustness of pose algorithms is to combine the camera with another form of sensor in order to compensate for the shortcomings of each technology.

The success of pose computation over time largely depends on the quality of the matching at the initialization stage. Indeed, the current image may be very different from the appearances described in the model both on the geometrical and the photometric sides. Research is thus conducted in the team on the use of probabilistic methods to establish robust correspondences of features. The use of *a contrario* methods has been investigated to achieve this aim [8]. We especially addressed the complex case of matching in scenes with repeated patterns which are common in urban scenes. We are also investigating the problem of matching images taken from very different viewpoints which is central for the re-localization issue in AR. Within the context of a scene model acquired with structure from motion techniques, we are currently investigating the use of viewpoint simulation in order to allow successful pose computation even if the considered image is far from the positions used to build the model [4].

Recently, the issue of tracking deformable objects has gained importance in the team. This topic is mainly addressed in the context of medical applications through the design of bio-mechanical models guided by visual features [1]. We have successfully investigated the use of such models in laparoscopy, with a vascularized model of the liver and with a hyper-elastic model for tongue tracking in ultrasound images. However, these results have been obtained so far in relatively controlled environments, with non pathological cases. When clinical routine applications are to be considered, many parameters and considerations need to be taken into account. Among the problems that need to be addressed are more realistic model representations, the specification of the range of physical parameters and the need to enforce the robustness of the tracking with respect to outliers, which are common in the interventional context.

3.2. Image-based Modeling

Modeling the scene is a fundamental issue in AR for many reasons. First, pose computation algorithms often use a model of the scene or at least some 3D knowledge on the scene. Second, effective AR systems require a model of the scene to support interactions between the virtual and the real objects such as occlusions, lighting reflections, contacts...in real-time. Unlike pose computation which has to be computed in a sequential way, scene modeling can be considered as an off-line or an on-line problem depending on the requirements of the targeted application. Interactive in-situ modeling techniques have thus been developed with the aim to enable the user to define what is relevant at the time the model is being built during the application. On the other hand, we also proposed off-line multimodal techniques, mainly dedicated to AR medical applications, with the aim to obtain realistic and possibly dynamic models of organs suitable for real-time simulation.

In-situ modeling
In-situ modeling allows a user to directly build a 3D model of his/her surrounding environment and verify the geometry against the physical world in real-time. This is of particular interest when using AR in unprepared environments or building scenes that either have an ephemeral existence (e.g., a film set) or cannot be accessed frequently (e.g., a nuclear power plant). We have especially investigated two systems, one based on the image content only and the other based on multiple data coming from different sensors (camera, inertial measurement unit, laser rangefinder). Both systems use the camera-mouse principle [6] (i.e., interactions are performed by aiming at the scene through a video camera) and both systems have been designed to acquire polygonal textured models, which are particularly useful for camera tracking and object insertion in AR.

Multimodal modeling for real-time simulation
With respect to classical AR applications, AR in medical context differs in the nature and the size of the data which are available: a large amount of multimodal data is acquired on the patient or possibly on the operating room through sensing technologies or various image acquisitions [3]. The challenge is to analyze these data, to extract interesting features, to fuse and to visualize this information in a proper way. Within the MAGRIT team, we address several key problems related to medical augmented environments. Being able to acquire multimodal data which are temporally synchronized and spatially registered is the first difficulty we face when considering medical AR. Another key requirement of AR medical systems is the availability of 3D (+t) models of the organ/patient built from images, to be overlaid onto the users' view of the environment.

Methods for multimodal modeling are strongly dependent on the image modalities and the organ specificities. We thus only address a restricted number of medical applications –interventional neuro-radiology, laparoscopic surgery– for which we have a strong expertise and close relationships with motivated clinicians. In these applications, our aim is to produce realistic models and then realistic simulations of the patient to be used for surgeon's training or patient's re-education/learning.

One of our main applications is about neuroradiology. For the last 20 years, we have been working in close collaboration with the neuroradiology laboratory (CHU-University Hospital of Nancy) and GE Healthcare. As several imaging modalities are now available in an intraoperative context (2D and 3D angiography, MRI, ...), our aim is to develop a multi-modality framework to help therapeutic decision and treatment.

We have mainly been interested in the effective use of a multimodality framework in the treatment of arteriovenous malformations (AVM) and aneurysms in the context of interventional neuroradiology. The goal of interventional gestures is to guide endoscopic tools towards the pathology with the aim to perform embolization of the AVM or to fill the aneurysmal cavity by placing coils. We have proposed and developed multimodality and augmented reality tools which make various image modalities (2D and 3D angiography, fluoroscopic images, MRI, ...) cooperate in order to help physicians in clinical routine. One of the successes of this collaboration is the implementation of the concept of *augmented fluoroscopy*, which helps the surgeon to guide endoscopic tools towards the pathology. Lately, in cooperation with the team MIMESIS, we have proposed new methods for implicit modeling of the vasculature with the aim of obtaining near real-time simulation of the coil deployment in the aneurysm [2]. These works open the way towards near real-time patient-based simulations of interventional gestures both for training and for planning.

3.3. Parameter estimation

Many problems in computer vision or image analysis can be formulated in terms of parameter estimation from image-based measurements. This is the case of many problems addressed in the team such as pose computation or image-guided estimation of 3D deformable models. Often traditional robust techniques which take into account the covariance on the measurements are sufficient to achieve reliable parameter estimation. However, depending on their number, their spatial distribution and the uncertainty on these measurements, some problems are very sensitive to noise and there is a considerable interest in considering how parameter estimation could be improved if additional information on the noise were available. Another common problem in our field of research is the need to estimate constitutive parameters of the models, such as (bio)-mechanical parameters for instance. Direct measurement methods are destructive and elaborating image based methods is thus highly desirable. Besides designing appropriate estimation algorithms, a fundamental question is to understand what group of parameters under study can be reliably estimated from a given experimental setup.

This line of research is relatively new in the team. One of the challenges is to improve image-based parameter estimation techniques considering sensor noise and specific image formation models. In a collaboration with the Pascal Institute (Clermont Ferrand), metrological performance enhancement for experimental solid mechanics has been addressed through the development of dedicated signal processing methods [7]. In the medical field, specific methods based on an adaptive evolutionary optimization strategy have been designed for estimating respiratory parameters [9]. In the context of designing realistic simulators for neuroradiology, we are now considering how parameters involved in the simulation could be adapted to fit real images.

MANAO Project-Team

3. Research Program

3.1. Related Scientific Domains

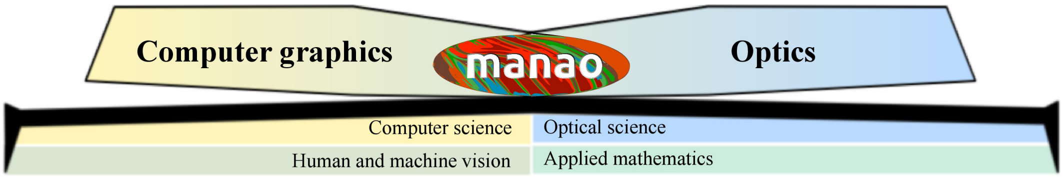


Figure 3. Related scientific domains of the MANAO project.

The *MANAO* project aims at studying, acquiring, modeling, and rendering the interactions between the three components that are light, shape, and matter from the viewpoint of an observer. As detailed more lengthily in the next section, such a work will be done using the following approach: first, we will tend to consider that these three components do not have strict frontiers when considering their impacts on the final observers; then, we will not only work in **computer graphics**, but also at the intersection of computer graphics and **optics**, exploring the mutual benefits that the two domains may provide. It is thus intrinsically a **transdisciplinary** project (as illustrated in Figure 3) and we expect results in both domains.

Thus, the proposed team-project aims at establishing a close collaboration between computer graphics (e.g., 3D modeling, geometry processing, shading techniques, vector graphics, and GPU programming) and optics (e.g., design of optical instruments, and theories of light propagation). The following examples illustrate the strengths of such a partnership. First, in addition to simpler radiative transfer equations [46] commonly used in computer graphics, research in the later will be based on state-of-the-art understanding of light propagation and scattering in real environments. Furthermore, research will rely on appropriate instrumentation expertise for the measurement [59], [60] and display [58] of the different phenomena. Reciprocally, optics researches may benefit from the expertise of computer graphics scientists on efficient processing to investigate interactive simulation, visualization, and design. Furthermore, new systems may be developed by unifying optical and digital processing capabilities. Currently, the scientific background of most of the team members is related to computer graphics and computer vision. A large part of their work have been focused on simulating and analyzing optical phenomena as well as in acquiring and visualizing them. Combined with the close collaboration with the optics laboratory LP2N (http://www.lp2n.fr) and with the students issued from the "Institut d'Optique" (http://www.institutoptique.fr), this background ensures that we can expect the following results from the project: the construction of a common vocabulary for tightening the collaboration between the two scientific domains and creating new research topics. By creating this context, we expect to attract (and even train) more trans-disciplinary researchers.

At the boundaries of the *MANAO* project lie issues in **human and machine vision**. We have to deal with the former whenever a human observer is taken into account. On one side, computational models of human vision are likely to guide the design of our algorithms. On the other side, the study of interactions between light, shape, and matter may shed some light on the understanding of visual perception. The same kind of connections are expected with machine vision. On the one hand, traditional computational methods for acquisition (such as photogrammetry) are going to be part of our toolbox. On the other hand, new display technologies (such as the ones used for augmented reality) are likely to benefit from our integrated approach and systems. In the *MANAO* project we are mostly users of results from human vision. When required, some experimentation might be done in collaboration with experts from this domain, like with the European PRISM project. For machine vision, provided the tight collaboration between optical and digital systems, research will be carried out inside the *MANAO* project.

Analysis and modeling rely on **tools from applied mathematics** such as differential and projective geometry, multi-scale models, frequency analysis [48] or differential analysis [85], linear and non-linear approximation techniques, stochastic and deterministic integrations, and linear algebra. We not only rely on classical tools, but also investigate and adapt recent techniques (e.g., improvements in approximation techniques), focusing on their ability to run on modern hardware: the development of our own tools (such as Eigen, see Section 6.3) is essential to control their performances and their abilities to be integrated into real-time solutions or into new instruments.

3.2. Research axes

The *MANAO* project is organized around four research axes that cover the large range of expertise of its members and associated members. We briefly introduce these four axes in this section. More details and their inter-influences that are illustrated in the Figure 2 will be given in the following sections.

Axis 1 is the theoretical foundation of the project. Its main goal is to increase the understanding of light, shape, and matter interactions by combining expertise from different domains: optics and human/machine vision for the analysis and computer graphics for the simulation aspect. The goal of our analyses is to identify the different layers/phenomena that compose the observed signal. In a second step, the development of physical simulations and numerical models of these identified phenomena is a way to validate the pertinence of the proposed decompositions.

In Axis 2, the final observers are mainly physical captors. Our goal is thus the development of new acquisition and display technologies that combine optical and digital processes in order to reach fast transfers between real and digital worlds, in order to increase the convergence of these two worlds.

Axes 3 and 4 focus on two aspects of computer graphics: rendering, visualization and illustration in Axis 3, and editing and modeling (content creation) in Axis 4. In these two axes, the final observers are mainly human users, either generic users or expert ones (e.g., archaeologist [89], computer graphics artists).

3.3. Axis 1: Analysis and Simulation

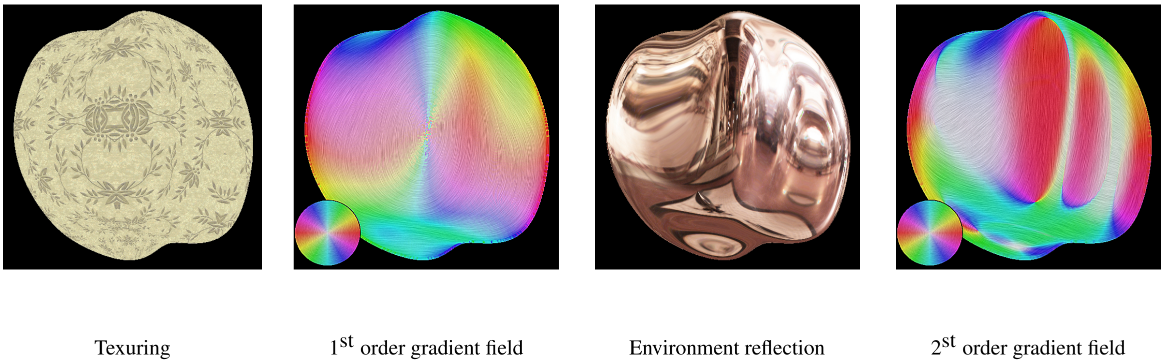
Challenge: Definition and understanding of phenomena resulting from interactions between light, shape, and matter as seen from an observer point of view.

Results: Theoretical tools and numerical models for analyzing and simulating the observed optical phenomena.

To reach the goals of the *MANAO* project, we need to **increase our understanding** of how light, shape, and matter act together in synergy and how the resulting signal is finally observed. For this purpose, we need to identify the different phenomena that may be captured by the targeted observers. This is the main objective of this research axis, and it is achieved by using three approaches: the simulation of interactions between light, shape, and matter, their analysis and the development of new numerical models. This resulting improved knowledge is a foundation for the researches done in the three other axes, and the simulation tools together with the numerical models serve the development of the joint optical/digital systems in Axis 2 and their validation.

One of the main and earliest goals in computer graphics is to faithfully reproduce the real world, focusing mainly on light transport. Compared to researchers in physics, researchers in computer graphics rely on a subset of physical laws (mostly radiative transfer and geometric optics), and their main concern is to efficiently use the limited available computational resources while developing as fast as possible algorithms. For this purpose, a large set of theoretical as well as computational tools has been introduced to take a **maximum benefit of hardware** specificities. These tools are often dedicated to specific phenomena (e.g., direct or indirect lighting, color bleeding, shadows, caustics). An efficiency-driven approach needs such a classification of light paths [55] in order to develop tailored strategies [101]. For instance, starting from simple direct lighting, more complex phenomena have been progressively introduced: first diffuse indirect illumination [53], [93], then more generic inter-reflections [62], [46] and volumetric scattering [90], [43]. Thanks to this search for efficiency and this classification, researchers in computer graphics have developed a now recognized expertise in fast-simulation of light propagation. Based on finite elements (radiosity techniques) or on unbiased Monte Carlo integration schemes (ray-tracing, particle-tracing, ...), the resulting algorithms and their combination are now sufficiently accurate to be used-back in physical simulations. The *MANAO* project will continue the search for **efficient and accurate simulation** techniques, but extending it from computer graphics to optics. Thanks to the close collaboration with scientific researchers from optics, new phenomena beyond radiative transfer and geometric optics will be explored.

Search for algorithmic efficiency and accuracy has to be done in parallel with **numerical models**. The goal of visual fidelity (generalized to accuracy from an observer point of view in the project) combined with the goal of efficiency leads to the development of alternative representations. For instance, common classical finite-element techniques compute only basis coefficients for each discretization element: the required discretization density would be too large and to computationally expensive to obtain detailed spatial variations and thus visual fidelity. Examples includes texture for decorrelating surface details from surface geometry and high-order wavelets for a multi-scale representation of lighting [42]. The numerical complexity explodes when considering directional properties of light transport such as radiance intensity (Watt per square meter and per steradian - $W.m^{-2}.sr^{-1}$), reducing the possibility to simulate or accurately represent some optical phenomena. For instance, Haar wavelets have been extended to the spherical domain [92] but are difficult to extend to non-piecewise-constant data [95]. More recently, researches prefer the use of Spherical Radial Basis Functions [98] or Spherical Harmonics [84]. For more complex data, such as reflective properties (e.g., BRDF [77], [63] - 4D), ray-space (e.g., Light-Field [73] - 4D), spatially varying reflective properties (6D - [88]), new models, and representations are still investigated such as rational functions [80] or dedicated models [31] and parameterizations [91], [96]. For each (newly) defined phenomena, we thus explore the space of possible numerical representations to determine the **most suited one for a given application**, like we have done for BRDF [80].


Texuring

1^{st} order gradient field

Environment reflection

2^{st} order gradient field

Figure 4. First-oder analysis [102] have shown that shading variations are caused by depth variations (first-order gradient field) and by normal variations (second-order fields). These fields are visualized using hue and saturation to indicate direction and magnitude of the flow respectively.

Before being able to simulate or to represent the different **observed phenomena**, we need to define and describe them. To understand the difference between an observed phenomenon and the classical light, shape, and matter decomposition, we can take the example of a highlight. Its observed shape (by a human user or a sensor) is the resulting process of the interaction of these three components, and can be simulated this way. However, this does not provide any intuitive understanding of their relative influence on the final shape: an artist will directly describe the resulting shape, and not each of the three properties. We thus want to decompose the observed signal into models for each scale that can be easily understandable, representable, and manipulable. For this purpose, we will rely on the **analysis** of the resulting interaction of light, shape, and matter as observed by a human or a physical sensor. We first consider this analysis from an **optical point of view**, trying to identify the different phenomena and their scale according to their mathematical properties (e.g., differential [85] and frequency analysis [48]). Such an approach has leaded us to exhibit the influence of surfaces flows (depth and normal gradients) into lighting pattern deformation (see Figure 4). For a **human observer**, this correspond to one recent trend in computer graphics that takes into account the human visual systems [49] both to evaluate the results and to guide the simulations.

3.4. Axis 2: From Acquisition to Display

Challenge: Convergence of optical and digital systems to blend real and virtual worlds.

Results: Instruments to acquire real world, to display virtual world, and to make both of them interact.

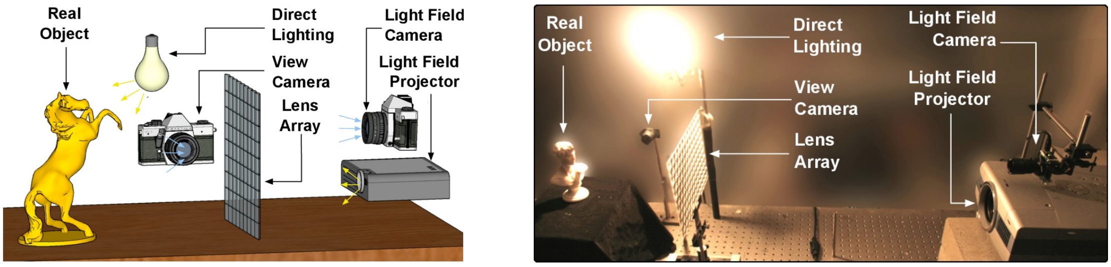


Figure 5. Light-Field transfer: global illumination between real and synthetic objects [41]

In this axis, we investigate *unified acquisition and display systems*, that is systems which combine optical instruments with digital processing. From digital to real, we investigate new display approaches [73], [58]. We consider projecting systems and surfaces [38], for personal use, virtual reality and augmented reality [33]. From the real world to the digital world, we favor direct measurements of parameters for models and representations, using (new) optical systems unless digitization is required [52], [51]. These resulting systems have to acquire the different phenomena described in Axis 1 and to display them, in an efficient manner [56], [32], [57], [60]. By efficient, we mean that we want to shorten the path between the real world and the virtual world by increasing the data bandwidth between the real (analog) and the virtual (digital) worlds, and by reducing the latency for real-time interactions (we have to prevent unnecessary conversions, and to reduce processing time). To reach this goal, the systems have to be designed as a whole, not by a simple concatenation of optical systems and digital processes, nor by considering each component independently [61].

To increase data bandwidth, one solution is to **parallelize more and more the physical systems**. One possible solution is to multiply the number of simultaneous acquisitions (e.g., simultaneous images from multiple viewpoints [60], [82]). Similarly, increasing the number of viewpoints is a way toward the creation of full 3D displays [73]. However, full acquisition or display of 3D real environments theoretically requires a continuous field of viewpoints, leading to huge data size. Despite the current belief that the increase of computational power will fill the missing gap, when it comes to visual or physical realism, if you double the processing power, people may want four times more accuracy, thus increasing data size as well. To reach the best performances, a trade-off has to be found between the amount of data required to represent accurately the reality and the amount of required processing. This trade-off may be achieved using **compressive sensing**. Compressive sensing is a new trend issued from the applied mathematics community that provides tools to accurately reconstruct a signal from a small set of measurements assuming that it is sparse in a transform domain (e.g., [81], [107]).

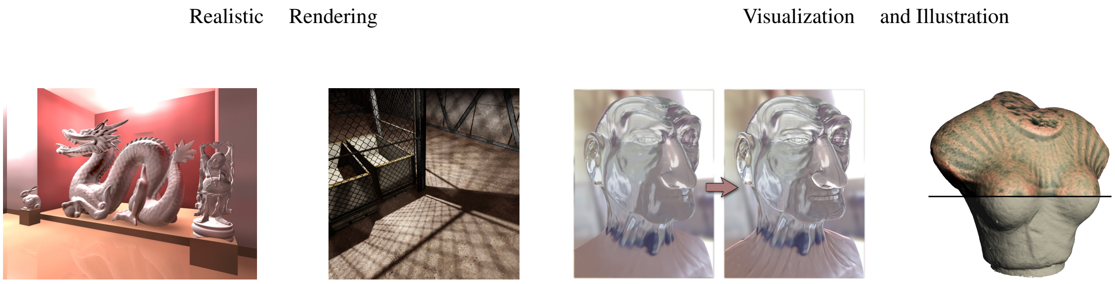
We prefer to achieve this goal by avoiding as much as possible the classical approach where acquisition is followed by a fitting step: this requires in general a large amount of measurements and the fitting itself may consume consequently too much memory and preprocessing time. By **preventing unnecessary conversion** through fitting techniques, such an approach increase the speed and reduce the data transfer for acquisition but also for display. One of the best recent examples is the work of Cossairt et al. [41]. The whole system is designed around a unique representation of the energy-field issued from (or leaving) a 3D object, either virtual or real: the Light-Field. A Light-Field encodes the light emitted in any direction from any position on an object. It is acquired thanks to a lens-array that leads to the capture of, and projection from, multiple simultaneous viewpoints. A unique representation is used for all the steps of this system. Lens-arrays, parallax barriers, and coded-aperture [70] are one of the key technologies to develop such acquisition (e.g., Light-Field camera [0] [61] and acquisition of light-sources [52]), projection systems (e.g., auto-stereoscopic displays). Such an approach is versatile and may be applied to improve classical optical instruments [68]. More generally, by designing unified optical and digital systems [78], it is possible to leverage the requirement of processing power, the memory footprint, and the cost of optical instruments.

Those are only some examples of what we investigate. We also consider the following approaches to develop new unified systems. First, similar to (and based on) the analysis goal of Axis 1, we have to take into account as much as possible the characteristics of the measurement setup. For instance, when fitting cannot be avoided, integrating them may improve both the processing efficiency and accuracy [80]. Second, we have to integrate signals from multiple sensors (such as GPS, accelerometer, ...) to prevent some computation (e.g., [71]). Finally, the experience of the group in surface modeling help the design of optical surfaces [64] for light sources or head-mounted displays.

3.5. Axis 3: Rendering, Visualization and Illustration

Challenge: How to offer the most legible signal to the final observer in real-time?

Results: High-level shading primitives, expressive rendering techniques for object depiction, real-time realistic rendering algorithms



(a) Global illumination [79] (b) Shadows [108] (c) Shape enhancement [104] (d) Shape depiction [30]

Figure 6. In the MANAO project, we are investigating rendering techniques from realistic solutions (e.g., inter-reflections (a) and shadows (b)) to more expressive ones (shape enhancement (c) with realistic style and shape depiction (d) with stylized style) for visualization.

The main goal of this axis is to offer to the final observer, in this case mostly a human user, the most legible signal in real-time. Thanks to the analysis and to the decomposition in different phenomena resulting from interactions between light, shape, and matter (Axis 1), and their perception, we can use them to convey essential information in the most pertinent way. Here, the word *pertinent* can take various forms depending on the application.

[0] Lytro, http://www.lytro.com/

In the context of scientific illustration and visualization, we are primarily interested in tools to convey shape or material characteristics of objects in animated 3D scenes. **Expressive rendering** techniques (see Figure 6 c,d) provide means for users to depict such features with their own style. To introduce our approach, we detail it from a shape-depiction point of view, domain where we have acquired a recognized expertise. Prior work in this area mostly focused on stylization primitives to achieve line-based rendering [105], [67] or stylized shading [36], [104] with various levels of abstraction. A clear representation of important 3D **object features** remains a major challenge for better shape depiction, stylization and abstraction purposes. Most existing representations provide only local properties (e.g., curvature), and thus lack characterization of broader shape features. To overcome this limitation, we are developing higher level descriptions of shape [29] with increased robustness to sparsity, noise, and outliers. This is achieved in close collaboration with Axis 1 by the use of higher-order local fitting methods, multi-scale analysis, and global regularization techniques. In order not to neglect the observer and the material characteristics of the objects, we couple this approach with an analysis of the appearance model. To our knowledge, this is an approach which has not been considered yet. This research direction is at the heart of the *MANAO* project, and has a strong connection with the analysis we plan to conduct in Axis 1. Material characteristics are always considered at the light ray level, but an understanding of **higher-level primitives** (like the shape of highlights and their motion) would help us to produce more legible renderings and permit novel stylizations; for instance, there is no method that is today able to create stylized renderings that follow the motion of highlights or shadows. We also believe such tools also play a fundamental role for geometry processing purposes (such as shape matching, reassembly, simplification), as well as for editing purposes as discussed in Axis 4.

In the context of **real-time photo-realistic rendering** ((see Figure 6 a,b), the challenge is to compute the most plausible images with minimal effort. During the last decade, a lot of work has been devoted to design approximate but real-time rendering algorithms of complex lighting phenomena such as soft-shadows [106], motion blur [48], depth of field [94], reflexions, refractions, and inter-reflexions. For most of these effects it becomes harder to discover fundamentally new and faster methods. On the other hand, we believe that significant speedup can still be achieved through more clever use of **massively parallel architectures** of the current and upcoming hardware, and/or through more clever tuning of the current algorithms. In particular, regarding the second aspect, we remark that most of the proposed algorithms depend on several parameters which can be used to **trade the speed over the quality**. Significant speed-up could thus be achieved by identifying effects that would be masked or facilitated and thus devote appropriate computational resources to the rendering [69], [47]. Indeed, the algorithm parameters controlling the quality vs speed are numerous without a direct mapping between their values and their effect. Moreover, their ideal values vary over space and time, and to be effective such an auto-tuning mechanism has to be extremely fast such that its cost is largely compensated by its gain. We believe that our various work on the analysis of the appearance such as in Axis 1 could be beneficial for such purpose too.

Realistic and real-time rendering is closely related to Axis 2: real-time rendering is a requirement to close the loop between real world and digital world. We have to thus develop algorithms and rendering primitives that allow the integration of the acquired data into real-time techniques. We have also to take care of that these real-time techniques have to work with new display systems. For instance, stereo, and more generally multi-view displays are based on the multiplication of simultaneous images. Brute force solutions consist in independent rendering pipeline for each viewpoint. A more energy-efficient solution would take advantages of the computation parts that may be factorized. Another example is the rendering techniques based on image processing, such as our work on augmented reality [40]. Independent image processing for each viewpoint may disturb the feeling of depth by introducing inconsistent information in each images. Finally, more dedicated displays [58] would require new rendering pipelines.

3.6. Axis 4: Editing and Modeling

Challenge: Editing and modeling appearance using drawing- or sculpting-like tools through high level representations.

Results: High-level primitives and hybrid representations for appearance and shape.

During the last decade, the domain of computer graphics has exhibited tremendous improvements in image quality, both for 2D applications and 3D engines. This is mainly due to the availability of an ever increasing amount of shape details, and sophisticated appearance effects including complex lighting environments. Unfortunately, with such a growth in visual richness, even so-called *vectorial* representations (e.g., subdivision surfaces, Bézier curves, gradient meshes, etc.) become very dense and unmanageable for the end user who has to deal with a huge mass of control points, color labels, and other parameters. This is becoming a major challenge, with a necessity for novel representations. This Axis is thus complementary of Axis 3: the focus is the development of primitives that are easy to use for modeling and editing.

More specifically, we plan to investigate *vectorial representations* that would be amenable to the production of rich shapes with a minimal set of primitives and/or parameters. To this end we plan to build upon our insights on dynamic local reconstruction techniques and implicit surfaces [4] [35]. When working in 3D, an interesting approach to produce detailed shapes is by means of procedural geometry generation. For instance, many natural phenomena like waves or clouds may be modeled using a combination of procedural functions. Turning such functions into triangle meshes (main rendering primitives of GPUs) is a tedious process that appears not to be necessary with an adapted vectorial shape representation where one could directly turn procedural functions into implicit geometric primitives. Since we want to prevent unnecessary conversions in the whole pipeline (here, between modeling and rendering steps), we will also consider *hybrid representations* mixing meshes and implicit representations. Such research has thus to be conducted while considering the associated editing tools as well as performance issues. It is indeed important to keep *real-time performance* (cf. Axis 2) throughout the interaction loop, from user inputs to display, via editing and rendering operations. Finally, it would be interesting to add *semantic information* into 2D or 3D geometric representations. Semantic geometry appears to be particularly useful for many applications such as the design of more efficient manipulation and animation tools, for automatic simplification and abstraction, or even for automatic indexing and searching. This constitutes a complementary but longer term research direction.

In the *MANAO* project, we want to investigate representations beyond the classical light, shape, and matter decomposition. We thus want to directly control the appearance of objects both in 2D and 3D applications (e.g., [99]): this is a core topic of computer graphics. When working with 2D vector graphics, digital artists must carefully set up color gradients and textures: examples range from the creation of 2D logos to the photo-realistic imitation of object materials. Classic vector primitives quickly become impractical for creating illusions of complex materials and illuminations, and as a result an increasing amount of time and skill is required. This is only for still images. For animations, vector graphics are only used to create legible appearances composed of simple lines and color gradients. There is thus a need for more complex primitives that are able to accommodate complex reflection or texture patterns, while keeping the ease of use of vector graphics. For instance, instead of drawing color gradients directly, it is more advantageous to draw flow lines that represent local surface concavities and convexities. Going through such an intermediate structure then allows to deform simple material gradients and textures in a coherent way (see Figure 7), and animate them all at once. The manipulation of 3D object materials also raises important issues. Most existing material models are tailored to faithfully reproduce physical behaviors, not to be *easily controllable* by artists. Therefore artists learn to tweak model parameters to satisfy the needs of a particular shading appearance, which can quickly become cumbersome as the complexity of a 3D scene increases. We believe that an alternative approach is required, whereby material appearance of an object in a typical lighting environment is directly input (e.g., painted or drawn), and adapted to match a plausible material behavior. This way, artists will be able to create their own appearance (e.g., by using our shading primitives [99]), and replicate it to novel illumination environments and 3D models. For this purpose, we will rely on the decompositions and tools issued from Axis 1.

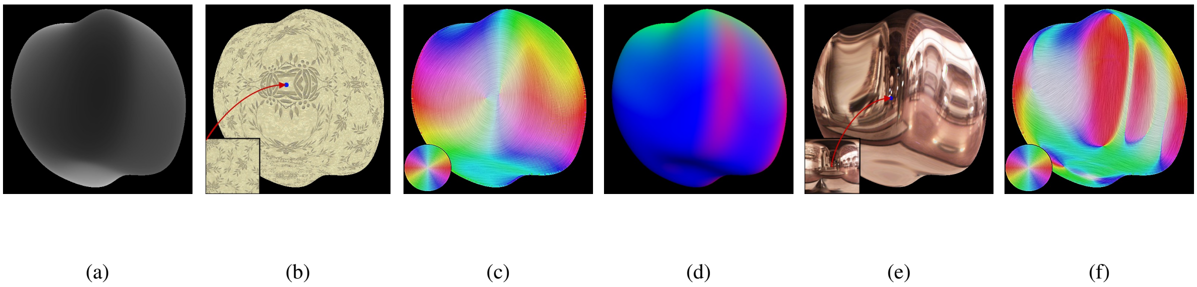


Figure 7. Based on our analysis [102] (Axis 1), we have designed a system that mimics texture (left) and shading (right) effects using image processing alone. It takes depth (a) and normal (d) images as input, and uses them to deform images (b-e) in ways that closely approximate surface flows (c-f). It provides a convincing, yet artistically controllable illusion of 3D shape conveyed through texture or shading cues.

MAVERICK Project-Team

3. Research Program

3.1. Introduction

The Maverick project-team aims at producing representations and algorithms for efficient, high-quality computer generation of pictures and animations through the study of four **research problems**:

- *Computer Visualization* where we take as input a large localized dataset and represent it in a way that will let an observer understand its key properties. Visualization can be used for data analysis, for the results of a simulation, for medical imaging data...
- *Expressive Rendering*, where we create an artistic representation of a virtual world. Expressive rendering corresponds to the generation of drawings or paintings of a virtual scene, but also to some areas of computational photography, where the picture is simplified in specific areas to focus the attention.
- *Illumination Simulation*, where we model the interaction of light with the objects in the scene, resulting in a photorealistic picture of the scene. Research include improving the quality and photorealism of pictures, including more complex effects such as depth-of-field or motion-blur. We are also working on accelerating the computations, both for real-time photorealistic rendering and offline, high-quality rendering.
- *Complex Scenes*, where we generate, manage, animate and render highly complex scenes, such as natural scenes with forests, rivers and oceans, but also large datasets for visualization. We are especially interested in interactive visualization of complex scenes, with all the associated challenges in terms of processing and memory bandwidth.

The fundamental research interest of Maverick is first, *understanding* what makes a picture useful, powerful and interesting for the user, and second *designing* algorithms to create and improve these pictures.

3.2. Research approaches

We will address these research problems through three interconnected research approaches:

3.2.1. Picture Impact

Our first research axis deals with the *impact* pictures have on the viewer, and how we can improve this impact. Our research here will target:

- *evaluating user response:* we need to evaluate how the viewers respond to the pictures and animations generated by our algorithms, through user studies, either asking the viewer about what he perceives in a picture or measuring how his body reacts (eye tracking, position tracking).
- *removing artefacts and discontinuities:* temporal and spatial discontinuities perturb viewer attention, distracting the viewer from the main message. These discontinuities occur during the picture creation process; finding and removing them is a difficult process.

3.2.2. Data Representation

The data we receive as input for picture generation is often unsuitable for interactive high-quality rendering: too many details, no spatial organisation... Similarly the pictures we produce or get as input for other algorithms can contain superfluous details.

One of our goals is to develop new data representations, adapted to our requirements for rendering. This includes fast access to the relevant information, but also access to the specific hierarchical level of information needed: we want to organize the data in hierarchical levels, pre-filter it so that sampling at a given level also gives information about the underlying levels. Our research for this axis include filtering, data abstraction, simplification and stylization.

The input data can be of any kind: geometric data, such as the model of an object, scientific data before visualization, pictures and photographs. It can be time-dependent or not; time-dependent data bring an additional level of challenge on the algorithm for fast updates.

3.2.3. Prediction and simulation

Our algorithms for generating pictures require computations: sampling, integration, simulation... These computations can be optimized if we already know the characteristics of the final picture. Our recent research has shown that it is possible to predict the local characteristics of a picture by studying the phenomena involved: the local complexity, the spatial variations, their direction...

Our goal is to develop new techniques for predicting the properties of a picture, and to adapt our image-generation algorithms to these properties, for example by sampling less in areas of low variation.

Our research problems and approaches are all cross-connected. Research on the *impact* of pictures is of interest in three different research problems: *Computer Visualization*, *Expressive rendering* and *Illumination Simulation*. Similarly, our research on *Illumination simulation* will use all three research approaches: impact, representations and prediction.

3.3. Cross-cutting research issues

Beyond the connections between our problems and research approaches, we are interested in several issues, which are present throughout all our research:

sampling is an ubiquitous process occurring in all our application domains, whether photorealistic rendering (*e.g.* photon mapping), expressive rendering (*e.g.* brush strokes), texturing, fluid simulation (Lagrangian methods), etc. When sampling and reconstructing a signal for picture generation, we have to ensure both coherence and homogeneity. By *coherence*, we mean not introducing spatial or temporal discontinuities in the reconstructed signal. By *homogeneity*, we mean that samples should be placed regularly in space and time. For a time-dependent signal, these requirements are conflicting with each other, opening new areas of research.

filtering is another ubiquitous process, occuring in all our application domains, whether in realistic rendering (*e.g.* for integrating height fields, normals, material properties), expressive rendering (*e.g.* for simplifying strokes), textures (through non-linearity and discontinuities). It is especially relevant when we are replacing a signal or data with a lower resolution (for hierarchical representation); this involves filtering the data with a reconstruction kernel, representing the transition between levels.

performance and scalability are also a common requirement for all our applications. We want our algorithms to be usable, which implies that they can be used on large and complex scenes, placing a great importance on scalability. For some applications, we target interactive and real-time applications, with an update frequency between 10 Hz and 120 Hz.

coherence and continuity in space and time is also a common requirement of realistic as well as expressive models which must be ensured despite contradictory requirements. We want to avoid flickering and aliasing.

animation: our input data is likely to be time-varying (*e.g.* animated geometry, physical simulation, time-dependent dataset). A common requirement for all our algorithms and data representation is that they must be compatible with animated data (fast updates for data structures, low latency algorithms...).

3.4. Methodology

Our research is guided by several methodological principles:

Experimentation: to find solutions and phenomenological models, we use experimentation, performing statistical measurements of how a system behaves. We then extract a model from the experimental data.

Validation: for each algorithm we develop, we look for experimental validation: measuring the behavior of the algorithm, how it scales, how it improves over the state-of-the-art... We also compare our algorithms to the exact solution. Validation is harder for some of our research domains, but it remains a key principle for us.

Reducing the complexity of the problem: the equations describing certain behaviors in image synthesis can have a large degree of complexity, precluding computations, especially in real time. This is true for physical simulation of fluids, tree growth, illumination simulation... We are looking for *emerging phenomena* and *phenomenological models* to describe them (see framed box "Emerging phenomena"). Using these, we simplify the theoretical models in a controlled way, to improve user interaction and accelerate the computations.

Transferring ideas from other domains: Computer Graphics is, by nature, at the interface of many research domains: physics for the behavior of light, applied mathematics for numerical simulation, biology, algorithmics... We import tools from all these domains, and keep looking for new tools and ideas.

Develop new fondamental tools: In situations where specific tools are required for a problem, we will proceed from a theoretical framework to develop them. These tools may in return have applications in other domains, and we are ready to disseminate them.

Collaborate with industrial partners: we have a long experiment of collaboration with industrial partners. These collaborations bring us new problems to solve, with short-term or medium-term transfert opportunities. When we cooperate with these partners, we have to find *what they need*, which can be very different from *what they want*, their expressed need.

MIMETIC Project-Team

3. Research Program

3.1. Biomechanics and Motion Control

Human motion control is a very complex phenomenon that involves several layered systems, as shown in Figure 3 . Each layer of this controller is responsible for dealing with perceptual stimuli in order to decide the actions that should be applied to the human body and his environment. Due to the intrinsic complexity of the information (internal representation of the body and mental state, external representation of the environment) used to perform this task, it is almost impossible to model all the possible states of the system. Even for simple problems, there generally exists an infinity of solutions. For example, from the biomechanical point of view, there are much more actuators (i.e. muscles) than degrees of freedom leading to an infinity of muscle activation patterns for a unique joint rotation. From the reactive point of view there exists an infinity of paths to avoid a given obstacle in navigation tasks. At each layer, the key problem is to understand how people select one solution among these infinite state spaces. Several scientific domains have addressed this problem with specific points of view, such as physiology, biomechanics, neurosciences and psychology.

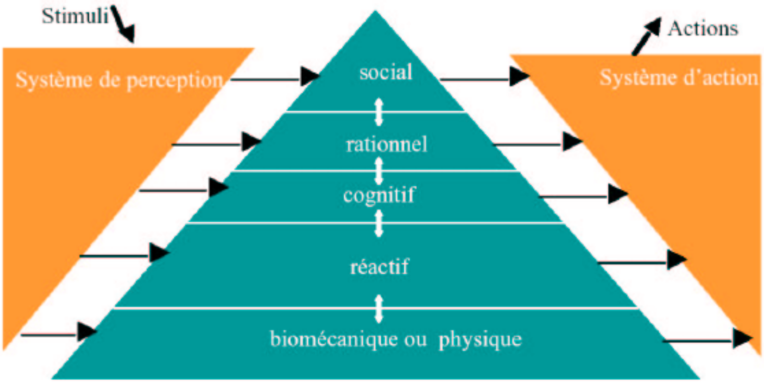


Figure 3. Layers of the motion control natural system in humans.

In biomechanics and physiology, researchers have proposed hypotheses based on accurate joint modeling (to identify the real anatomical rotational axes), energy minimization, force and torques minimization, comfort maximization (i.e. avoiding joint limits), and physiological limitations in muscle force production. All these constraints have been used in optimal controllers to simulate natural motions. The main problem is thus to define how these constraints are composed altogether such as searching the weights used to linearly combine these criteria in order to generate a natural motion. Musculoskeletal models are stereotyped examples for which there exists an infinity of muscle activation patterns, especially when dealing with antagonist muscles. An unresolved problem is to define how to use the above criteria to retrieve the actual activation patterns, while optimization approaches still leads to unrealistic ones. It is still an open problem that will require multidisciplinary skills including computer simulation, constraint solving, biomechanics, optimal control, physiology and neurosciences.

In neurosciences, researchers have proposed other theories, such as coordination patterns between joints driven by simplifications of the variables used to control the motion. The key idea is to assume that instead of controlling all the degrees of freedom, people control higher level variables which correspond to combinations of joint angles. In walking, data reduction techniques such as Principal Component Analysis have shown that lower-limb joint angles are generally projected on a unique plane whose angle in the state space is associated with energy expenditure. Although knowledge exists for specific motions, such as locomotion or grasping, this type of approach is still difficult to generalize. The key problem is that many variables are coupled and it is very difficult to objectively study the behavior of a unique variable in various motor tasks. Computer simulation is a promising method to evaluate such type of assumptions as it enables to accurately control all the variables and to check if it leads to natural movements.

Neurosciences also address the problem of coupling perception and action by providing control laws based on visual cues (or any other senses), such as determining how the optical flow is used to control direction in navigation tasks, while dealing with collision avoidance or interception. Coupling of the control variables is enhanced in this case as the state of the body is enriched by the large amount of external information that the subject can use. Virtual environments inhabited with autonomous characters whose behavior is driven by motion control assumptions is a promising approach to solve this problem. For example, an interesting problem in this field is navigation in an environment inhabited with other people. Typically, avoiding static obstacles together with other people displacing into the environment is a combinatory problem that strongly relies on the coupling between perception and action.

One of the main objectives of MimeTIC is to enhance knowledge on human motion control by developing innovative experiments based on computer simulation and immersive environments. To this end, designing experimental protocols is a key point and some of the researchers in MimeTIC have developed this skill in biomechanics and perception-action coupling. Associating these researchers to experts in virtual human simulation, computational geometry and constraints solving enable us to contribute to enhance fundamental knowledge in human motion control.

3.2. Experiments in Virtual Reality

Understanding interactions between humans is very challenging because it addresses many complex phenomena including perception, decision-making, cognition and social behaviors. Moreover, all these phenomena are difficult to isolate in real situations, and it is therefore very complex to understand their individual influence on these human interactions. It is then necessary to find an alternative solution that can standardize the experiments and that allows the modification of only one parameter at a time. Video was first used since the displayed experiment is perfectly repeatable and cut-offs (stop the video at a specific time before its end) allow having temporal information. Nevertheless, the absence of adapted viewpoint and stereoscopic vision does not provide depth information that are very meaningful. Moreover, during video recording session, the real human is acting in front of a camera and not of an opponent. The interaction is then not a real interaction between humans.

Virtual Reality (VR) systems allow full standardization of the experimental situations and the complete control of the virtual environment. It is then possible to modify only one parameter at a time and to observe its influence on the perception of the immersed subject. VR can then be used to understand what information is picked up to make a decision. Moreover, cut-offs can also be used to obtain temporal information about when information is picked up. When the subject can moreover react as in a real situation, his movement (captured in real time) provides information about his reactions to the modified parameter. Not only is the perception studied, but the complete perception-action loop. Perception and action are indeed coupled and influence each other as suggested by Gibson in 1979.

Finally, VR allows the validation of the virtual human models. Some models are indeed based on the interaction between the virtual character and the other humans, such as a walking model. In that case, there are two ways to validate it. First, they can be compared to real data (e.g. real trajectories of pedestrians). But such data are not always available and are difficult to get. The alternative solution is then to use VR. The validation of the realism of the model is then done by immersing a real subject in a virtual environment in which a virtual character is controlled by the model. Its evaluation is then deduced from how the immersed subject reacts when interacting with the model and how realistic he feels the virtual character is.

3.3. Computational Geometry

Computational geometry is a branch of computer science devoted to the study of algorithms which can be stated in terms of geometry. It aims at studying algorithms for combinatorial, topological and metric problems concerning sets of points in Euclidian spaces. Combinatorial computational geometry focuses on three main problem classes: static problems, geometric query problems and dynamic problems.

In static problems, some inputs are given and the corresponding outputs need to be constructed or found. Such problems include linear programming, Delaunay triangulations, and Euclidian shortest paths for instance. In geometric query problems, commonly known as geometric search problems, the input consists of two parts: the search space part and the query part, which varies over the problem instances. The search space typically needs to be preprocessed, in a way that multiple queries can be answered efficiently. Some typical problems are range searching, point location in a portioned space, or nearest neighbor queries. In dynamic problems, the goal is to find an efficient algorithm for finding a solution repeatedly after each incremental modification of the input data (addition, deletion or motion of input geometric elements). Algorithms for problems of this type typically involve dynamic data structures. Both of previous problem types can be converted into a dynamic problem, for instance, maintaining a Delaunay triangulation between moving points.

In this context, distance geometry relies solely on distances, instead of points and lines, as in classical geometry. Various applications lead to the definition of problems that can be formulated as a distance geometry, including sensor network localization, robot coordination, the identification of molecular conformations, or as in the context of MimeTIC relations between objects in virtual scenes (e.g., distances between body segments, agents, or cameras). In recent years, scientific research has been oriented to the assumptions allowing for discretizing the search space of a given distance geometry problem. The discretization (which is exact in some situations) allows to conceive ad-hoc and efficient algorithms, and for enumerating the entire solution set of a given instance.

The Mimetic team works on problems such as crowd simulation, spatial analysis, path and motion planning in static and dynamic environments, camera planning with visibility constraints for instance. The core of those problems, by nature, relies on problems and techniques belonging to computational geometry. Proposed models pay attention to algorithms complexity to be compatible with performance constraints imposed by interactive applications.

MINT Project-Team

3. Research Program

3.1. Human-Computer Interaction

The scientific approach that we follow considers user interfaces as means, not an end: our focus is not on interfaces, but on interaction considered as a phenomenon between a person and a computing system [26]. We *observe* this phenomenon in order to understand it, i.e. *describe* it and possibly *explain* it, and we look for ways to significantly *improve* it. HCI borrows its methods from various disciplines, including Computer Science, Psychology, Ethnography and Design. Participatory design methods can help determine users' problems and needs and generate new ideas, for example [30]. Rapid and iterative prototyping techniques allow to decide between alternative solutions [27]. Controlled studies based on experimental or quasi-experimental designs can then be used to evaluate the chosen solutions [32]. One of the main difficulties of HCI research is the doubly changing nature of the studied phenomenon: people can both adapt to the system and at the same time adapt it for their own specific purposes [29]. As these purposes are usually difficult to anticipate, we regularly *create* new versions of the systems we develop to take into account new theoretical and empirical knowledge. We also seek to *integrate* this knowledge in theoretical frameworks and software tools to disseminate it.

3.2. Numerical and algorithmic real-time gesture analysis

Whatever is the interface, user provides some curves, defined over time, to the application. The curves constitute a gesture (positional information, yet may also include pressure). Depending on the hardware input, such a gesture may be either continuous (e.g. data-glove), or not (e.g. multi-touch screens). User gesture can be multi-variate (several fingers captured at the same time, combined into a single gesture, possibly involving two hands, maybe more in the context of co-located collaboration), that we would like, at higher-level, to be structured in time from simple elements in order to create specific command combinations. One of the scientific foundations of the research project is an algorithmic and numerical study of gesture, which we classify into three points:

- *clustering*, that takes into account intrinsic structure of gesture (multi-finger/multi-hand/multi-user aspects), as a lower-level treatment for further use of gesture by application;
- *recognition*, that identifies some semantic from gesture, that can be further used for application control (as command input). We consider in this topic multi-finger gestures, two-handed gestures, gesture for collaboration, on which very few has been done so far to our knowledge. On the contrary, in the case of single gesture case (i.e. one single point moving over time in a continuous manner), numerous studies have been proposed in the current literature, and interestingly, are of interest in several communities: HMM [33], Dynamic Time Warping [35] are well-known methods for computer-vision community, and hand-writing recognition. In the computer graphics community, statistical classification using geometric descriptors has previously been used [31]; in the Human-Computer interaction community, some simple (and easy to implement) methods have been proposed, that provide a very good compromise between technical complexity and practical efficiency [34].
- *mapping to application*, that studies how to link gesture inputs to application. This ranges from transfer function that is classically involved in pointing tasks [28], to the question to know how to link gesture analysis and recognition to the algorithmic of application content, with specific reference examples.

We ground our activity on the topic of numerical algorithm, expertise that has been previously achieved by team members in the physical simulation community (within which we think that aspects such as elastic deformation energies evaluation, simulation of rigid bodies composed of unstructured particles, constraint-based animation... will bring up interesting and novel insights within HCI community).

3.3. Design and control of haptic devices

Our scientific approach in the design and control of haptic devices is focused on the interaction forces between the user and the device. We search of controlling them, as precisely as possible. This leads to different designs compared to other systems which control the deformation instead. The research is carried out in three steps:

- *identification:* we measure the forces which occur during the exploration of a real object, for example a surface for tactile purposes. We then analyse the record to deduce the key components – *on user's point of view* – of the interaction forces.
- *design:* we propose new designs of haptic devices, based on our knowledge of the key components of the interaction forces. For example, coupling tactile and kinesthetic feedback is a promising design to achieve a good simulation of actual surfaces. Our goal is to find designs which lead to compact systems, and which can stand close to a computer in a desktop environment.
- *control:* we have to supply the device with the good electrical signals to accurately output the good forces.

Mjolnir Team

3. Research Program

3.1. Introduction

Our research program is organized around three main themes: leveraging human control skills, leveraging human perceptual skills, and leveraging human learning skills.

3.2. Leveraging human control skills

Our group has developed a unique and recognized expertise in *transfer functions*, i.e. the algorithmic transformations of raw user input for system use. Transfer functions define how user actions are taken into account by the system. They can make a task easier or impossible and thus largely condition user performance, no matter the criteria (speed, accuracy, comfort, fatigue, etc). Ideally, the transfer function should be chosen or tuned to match the interaction context. Yet the question of how to design a function to maximize one or more criteria in a given context remains an open one, and on-demand adaptation is difficult because functions are usually implemented at the lowest possible level to avoid latency problems. Latency management and transfer function design are two problems that require cross examination to improve human performance with interactive systems. Both also contribute to the senses of *initiation* and *control*, two crucial component of the sense of *agency* [51]. Our ultimate goal on these topics is to adapt the transfer function to the user and task in order to support stable and appropriate control. To achieve this, we investigate combinations of low-level (embedded) and high-level (application) ways to take user capabilities and task characteristics into account and reduce or compensate for latency in different contexts, e.g. using a mouse or a touchpad, a touch-screen, an optical finger navigation device or a brain-computer interface.

3.3. Leveraging human perceptual skills

Our work under this theme concerns the physicality of human-computer interaction, with a focus on haptic perception and related technologies, and the perception of animated displays.

Vibrators have long been used to provide basic kinesthetic feedback. Other piezoceramic and electro-active polymer technologies make it possible to support programmable friction or emboss a surface, and thin, organic technologies should soon provide transparent and conformable, flexible or stretchable substrates. We want to study the use of these different technologies for static and dynamic haptic feedback from both an engineering and an HCI perspective. We want to develop the tools and knowledge required to facilitate and inform the design of future haptic interactions taking best advantage of the different technologies.

Animations are increasingly common in graphical interfaces. Beyond their compelling nature, they are powerful tools that can be used to depict dynamic data, to help understand time-varying behaviors, to communicate a particular message or to capture attention. Yet despite their popularity, they are still largely under-comprehended as cognitive aids. While best practices provide useful directions, very little empirical research examine different types of animation, and their actual benefits and limitations remain to be determined. We want to increase current knowledge and develop the tools required to best take advantage of them.

3.4. Leveraging human learning skills

By looking at ways to leverage human control and perceptual skills, the research yet proposed mainly aims at improving perception-action coupling to better support transparent use. This third research theme addresses the different and orthogonal topic of skill acquisition and improvement. We want to move away from the usual binary distinction between “novices” and “experts” and explore means to promote and assist digital skill development in a more progressive fashion. We are interested in means to support the analytic use of computing tools. We want to help people become aware of the particular ways they use their tools, the other ways that exist for the things they do, and the other things they might do. We want to help them increase their performance by adjusting their current ways of doing, by providing new and more efficient ways, and by facilitating transitions from one way to another. We are also interested in means to foster reflection among users and facilitate the dissemination of best practices.

MORPHEO Project-Team

3. Research Program

3.1. Shape Acquisition

Multiple camera setups allow to acquire shapes, i.e. geometry, as well as their appearances, i.e. photometry, with a reasonable level of precision. However fundamental limitations still exist, in particular today's state-of-the-art approaches do not fully exploit the redundancy of information over temporal sequences of visual observations. Despite an increasing interest of the computer vision communities in the past years, the problem is still far from solved other than in specific situations with restrictive assumptions and configurations. Our goal in this research axis is to fully leverage temporal aspects of the acquisition process and to open the acquisition process to different modalities, in particular Xrays.

3.2. Generative / discriminative inference

Acquisition of 4D Models can often be conveniently formulated as an estimation or learning problem. Various generative models can be proposed for the problems of shape and appearance modeling over time sequences, and motion segmentation. The idea of these generative models is to predict the noisy measurements (e.g. pixel values, measured 3D points or speed quantities) from a set of parameters describing the unobserved scene state (e.g. shape and appearance), which in turn can be inverted with various inference algorithms. The advantages of this type of modeling are numerous to deal with noisy measurements, explicitly model dependencies between model parameters, hidden variables and observed quantities, and relevant priors over parameters; sensor models for different modalities can also easily be seamlessly integrated and jointly used, which remains central to our goals. A limitation of such algorithms is that classical algorithms to solve them rely on local iterative convergence schemes subject to local minima, or global restart schemes which avert this problem but with a significant computational penalty. This is why we also consider discriminative and deep learning approaches, which allow to formulate the parameter estimation as a direct regression from input quantities or pixel values, whose parameters are learned given a training set. This has the advantage of directly computing a solution from inputs, with robustness and speed benefits, as a standalone estimation algorithm or to initialize local convergence schemes based on generative modeling. A number of the approaches we propose thus leverage the advantages of both generative and such discriminative approaches.

3.3. Shape Analysis

Shape analysis has received much attention from the scientific community and recovering the intrinsic nature of shapes is currently an active research domain. Of particular interest is the study of human and animal shapes and their associated articulated underlying structures, i.e. skeletons, since applications are numerous, either in the entertainment industry or for medical applications, among others. Our main goals in this research axis are : the understanding of a shape's global structure, and a pose-independent classification of shapes.

3.4. Shape Tracking

Recovering the temporal evolution of a deformable surface is a fundamental task in computer vision, with a large variety of applications ranging from the motion capture of articulated shapes, such as human bodies, to the deformation of complex surfaces such as clothes. Methods that solve for this problem usually infer surface evolutions from motion or geometric cues. This information can be provided by motion capture systems or one of the numerous available static 3D acquisition modalities. In this inference, methods are faced with the challenging estimation of the time-consistent deformation of a surface from cues that can be sparse and noisy. Such an estimation is an ill posed problem that requires prior knowledge on the deformation to be introduced in order to limit the range of possible solutions. Our goal is to devise robust and accurate solutions based on new deformation models that fully exploit the geometric and photometric information available.

3.5. Dynamic Motion Modeling

Multiple views systems can significantly change the paradigm of motion capture. Traditional motion capture systems provide 3D trajectories of a sparse set of markers fixed on the subject. These trajectories can be transformed into motion parameters on articulated limbs with the help of prior models of the skeletal structure. However, such skeletal models are mainly robotical abstractions that do not describe the true morphology and anatomical motions of humans and animals. On the other hand, 4D models (temporally consistent mesh sequences) provide dense motion information on body's shape while requiring less prior assumption. They represent therefore a new rich source of information on human and animal shape movements. The analysis of such data has already received some attention but most existing works model motion through static poses and do not consider yet dynamic information. Such information (e.g. trajectories and speed) is anyway required to analyse walking or running sequences. We will investigate this research direction with the aim to propose and study new dynamic models.

3.6. Shape Animation

3D animation is a crucial part of digital media production with numerous applications, in particular in the game and motion picture industry. Recent evolutions in computer animation consider real videos for both the creation and the animation of characters. The advantage of this strategy is twofold: it reduces the creation cost and increases realism by considering only real data. Furthermore, it allows to create new motions, for real characters, by recombining recorded elementary movements. In addition to enable new media contents to be produced, it also allows to automatically extend moving shape datasets with fully controllable new motions. This ability appears to be of great importance with the recent advent of deep learning techniques and the associated need for large learning datasets. In this research direction, we will investigate how to create new dynamic scenes using recorded events.

MULTISPEECH Project-Team

3. Research Program

3.1. Explicit Modeling of Speech Production and Perception

Speech signals are the consequence of the deformation of the vocal tract under the effect of the movements of the articulators (jaw, lips, tongue, ...) to modulate the excitation signal produced by the vocal cords or air turbulence. These deformations are visible on the face (lips, cheeks, jaw) through the coordination of different orofacial muscles and skin deformation induced by the latter. These deformations may also express different emotions. We should note that human speech expresses more than just phonetic content, to be able to communicate effectively. In this project, we address the different aspects related to speech production from the modeling of the vocal tract up to the production of expressive audiovisual speech. Phonetic contrasts used by the phonological system of any language result from constraints imposed by the nature of the human speech production apparatus. For a given language these contrasts are organized so as to guarantee that human listeners can identify (categorize) sounds robustly. The study of the categorization of sounds and prosody thus provides a complementary view on speech signals by focusing on the discrimination of sounds by humans, particularly in the context of language learning.

3.1.1. Articulatory modeling

Modeling speech production is a major issue in speech sciences. Acoustic simulation makes the link between articulatory and acoustic domains. Unfortunately this link cannot be fully exploited because there is almost always an acoustic mismatch between natural and synthetic speech generated with an articulatory model approximating the vocal tract. However, the respective effects of the geometric approximation, of the fact of neglecting some cavities in the simulation, of the imprecision of some physical constants and of the dimensionality of the acoustic simulation are still unknown. Hence, the first objective is to investigate the origin of the acoustic mismatch by designing more precise articulatory models, developing new methods to acquire tridimensional Magnetic Resonance Imaging (MRI) data of the entire vocal tract together with denoised speech signals, and evaluating several approaches of acoustic simulation. The articulatory data acquisition relies on a head-neck antenna at Nancy Hospital to acquire MRI of the vocal tract, and on the articulograph Carstens AG501 available in the laboratory.

Up to now, acoustic-to-articulatory inversion has been addressed as an instantaneous problem, articulatory gestures being recovered by concatenating local solutions. The second objective is thus to investigate how more elaborated strategies (a syllabus of primitive gestures, articulatory targets. . .) can be incorporated in the acoustic-to-articulatory inversion algorithms to take into account dynamic aspects.

3.1.2. Expressive acoustic-visual synthesis

Speech is considered as a bimodal communication means; the first modality is audio, provided by acoustic speech signals and the second one is visual, provided by the face of the speaker. In our approach, the Acoustic-Visual Text-To-Speech synthesis (AV-TTS) is performed simultaneously with respect to its acoustic and visible components, by considering a bimodal signal comprising both acoustic and visual channels. A first AV-TTS system has been developed resulting in a talking head; the system relied on 3D-visual data and on an extension of our acoustic-unit concatenation text-to-speech synthesis system (SoJA). An important goal is to provide an audiovisual synthesis that is intelligible, both acoustically and visually. Thus, we continue working on adding visible components of the head through a tongue model and a lip model. We will also improve the TTS engine to increase the accuracy of the unit selection simultaneously into the acoustic and visual domains. To acquire the facial data, we consider using a marker-less motion capture system using a kinect-like system with a face tracking software, which constitutes a relatively low-cost alternative to the Vicon system.

Another challenging research goal is to add expressivity in the AV-TTS. The expressivity comes through the acoustic signal (prosody aspects) and also through head and eyebrow movements. One objective is to add a prosodic component in the TTS engine in order to take into account some prosodic entities such as emphasis (to highlight some important key words). One intended approach will be to explore an expressivity measure at sound, syllable and/or sentence levels that describes the degree of perception or realization of an expression/emotion (audio and 3D domain). Such measures will be used as criteria in the selection process of the synthesis system. To tackle the expressivity issue we will also investigate Hidden Markov Model (HMM) based synthesis which allows for easy adaptation of the system to available data and to various conditions.

3.1.3. Categorization of sounds and prosody for native and non-native speech

Discriminating speech sounds and prosodic patterns is the keystone of language learning whether in the mother tongue or in a second language. This issue is associated with the emergence of phonetic categories, i.e., classes of sounds related to phonemes and prosodic patterns. The study of categorization is concerned not only with acoustic modeling but also with speech perception and phonology. Foreign language learning raises the issue of categorizing phonemes of the second language given the phonetic categories of the mother tongue. Thus, studies on the emergence of new categories, whether in the mother tongue (for people with language deficiencies) or in a second language, must rely upon studies on native and non-native acoustic realizations of speech sounds and prosody, and on perceptual experiments. Concerning prosody, studies are focused on native and non-native realizations of modalities (e.g., question, affirmation, command, ...), as well as non-native realizations of lexical accents and focus (emphasis).

For language learning, the analysis of the prosody and of the acoustic realization of the sounds aims at providing automatic feedback to language learners with respect to acquisition of prosody as well as acquisition of a correct pronunciation of the sounds of the foreign language. Concerning the mother tongue we are interested in the monitoring of the process of sound categorization in the long term (mainly at primary school) and its relation with the learning of reading and writing skills [7], especially for children with language deficiencies.

3.2. Statistical Modeling of Speech

Whereas the first research direction deals with the physical aspects of speech and its explicit modeling, this second research direction investigates statistical models for speech data. Acoustic models are used to represent the pronunciation of the sounds or other acoustic events such as noise. Whether they are used for source separation, for speech recognition, for speech transcription, or for speech synthesis, the achieved performance strongly depends on the accuracy of these models. At the linguistic level, MULTISPEECH investigates models for handling the context (beyond the few preceding words currently handled by the n-gram models) and evolutive lexicons necessary when dealing with diachronic audio documents. Statistical approaches are also useful for generating speech signals. Along this direction, MULTISPEECH considers voice transformation techniques, with their application to pathological voices, and statistical speech synthesis applied to expressive multimodal speech synthesis.

3.2.1. Source separation

Acoustic modeling is a key issue for automatic speech recognition. Despite the progress made for many years, current speech recognition applications rely on strong constraints (close-talk microphone, limited vocabulary, or restricted syntax) to achieve acceptable performance. The quality of the input speech signals is particularly important and performance degrades quickly with noisy signals. Accurate signal enhancement techniques are therefore essential to increase the robustness of both automatic speech recognition and speech-text alignment systems to noise and non-speech events.

In MULTISPEECH, focus is set on source separation techniques using multiple microphones and/or models of non-speech events. Some of the challenges include getting the most of the new modeling frameworks based on alpha-stable distributions and deep neural networks, combining them with established spatial filtering approaches, modeling more complex properties of speech and audio sources (phase, inter-frame and inter-frequency properties), and exploiting large data sets of speech, noise, and acoustic impulse responses to automatically discover new models. Beyond the definition of such models, the difficulty will be to design scalable estimation algorithms robust to overfitting, integrate them into the recently developed FASST [6] and KAM software frameworks if relevant, and develop new software frameworks otherwise.

3.2.2. Linguistic modeling

MULTISPEECH investigates lexical and language models in speech recognition with a focus on improving the processing of proper names and of spontaneous speech. Proper names are relevant keys in information indexing, but are a real problem in transcribing many diachronic spoken documents which refer to data, especially proper names, that evolve over time. This leads to the challenge of dynamically adjusting lexicons and language models through the use of the context of the documents or of some relevant external information. We also investigate language models defined on a continuous space (through neural network based approaches) in order to achieve a better generalization on unseen data, and to model long-term dependencies. We also want to introduce into these models additional relevant information such as linguistic features, semantic relation, topic or user-dependent information.

Other topics are spontaneous speech and pronunciation lexicons. Spontaneous speech utterances are often ill-formed and frequently contain disfluencies (hesitations, repetitions, ...) that degrade speech recognition performance. Hence the objective of improving the modeling of disfluencies and of spontaneous speech pronunciation variants. Attention will also be set on pronunciation lexicons with respect to non-native speech and foreign names. Non-native pronunciation variants have to take into account frequent mis-pronunciations due to differences between mother tongue and target language phoneme inventories. Proper name pronunciation variants are a similar problem where difficulties are mainly observed for names of foreign origin that can be pronounced either in a French way or kept close to foreign origin native pronunciation.

3.2.3. Speech generation by statistical methods

Over the last few years statistical speech synthesis has emerged as an alternative to corpus-based speech synthesis. The announced advantages of the statistical speech synthesis are the possibility to deal with small amounts of speech resources and the flexibility for adapting models (for new emotions or new speakers), however, the quality is not as good as that of the concatenation-based speech synthesis. MULTISPEECH will focus on a hybrid approach, combining corpus-based synthesis, for its high-quality speech signal output, and HMM-based speech synthesis for its flexibility to drive selection, and the main challenge will be on its application to producing expressive audio-visual speech.

Moreover, in the context of acoustic feedback in foreign language learning, voice modification approaches are investigated to modify the learner's (or teacher's) voice in order to emphasize the difference between the learner's acoustic realization and the expected realization.

3.3. Uncertainty Estimation and Exploitation in Speech Processing

This axis focuses on the uncertainty associated with some processing steps. Uncertainty stems from the high variability of speech signals and from imperfect models. For example, enhanced speech signals resulting from source separation are not exactly the clean original speech signals. Words or phonemes resulting from automatic speech recognition contain errors, and the phone boundaries resulting from an automatic speech-text alignment are not always correct, especially in acoustically degraded conditions. Hence it is important to know the reliability of the results and/or to estimate the uncertainty of the results.

3.3.1. Uncertainty and acoustic modeling

Because small distortions in the separated source signals can translate into large distortions in the cepstral features used for speech recognition, this limits the recognition performance on noisy data. One way to address this issue is to estimate the uncertainty of the separated sources in the form of their posterior distribution and to propagate this distribution, instead of a point estimate, through the subsequent feature extraction and speech decoding stages. Although major improvements have been demonstrated in proof-of-concept experiments using knowledge of the true uncertainty, accurate uncertainty estimation and propagation remains an open issue.

MULTISPEECH seeks to provide more accurate estimates of the posterior distribution of the separated source signals accounting for, e.g., posterior correlations over time and frequency which have not been considered so far. The framework of variational Bayesian (VB) inference appears to be a promising direction. Mappings learned on training data and fusion of multiple uncertainty estimators are also explored. The estimated uncertainties are then exploited for acoustic modeling in speech recognition and, in the future, also for speech-text alignment. This approach may later be extended to the estimation of the resulting uncertainty of the acoustic model parameters and of the acoustic scores themselves.

3.3.2. Uncertainty and phonetic segmentation

The accuracy of the phonetic segmentation is important in several cases, as for example for the computation of prosodic features, for avoiding incorrect feedback to the learner in computer assisted foreign language learning, or for the post-synchronization of speech with face/lip images. Currently the phonetic boundaries obtained are quite correct on good quality speech, but the precision degrades significantly on noisy and non-native speech. Phonetic segmentation aspects will be investigated, both in speech recognition (i.e., spoken text unknown) and in forced alignment (i.e., when the spoken text is known).

In the same way that combining several speech recognition outputs leads to improved speech recognition performance, MULTISPEECH will investigate the combination of several speech-text alignments as a way of improving the quality of speech-text alignment and of determining which phonetic boundaries are reliable and which ones are not, and also for estimating the uncertainty of the boundaries. Knowing the reliability of the boundaries will also be useful when segmenting speech corpora; this will help deciding which parts of the corpora need to be manually checked and corrected without an exhaustive checking of the whole corpus.

3.3.3. Uncertainty and prosody

Prosody information is also investigated as a means for structuring speech data (determining sentence boundaries, punctuation. . .) possibly in addition to syntactic dependencies. Structuring automatic transcription output is important for further exploitation of the transcription results such as easier reading after the addition of punctuation, or exploitation of full sentences in automatic translation. Prosody information is also necessary for determining the modality of the utterance (question or not), as well as determining accented words.

Prosody information comes from the fundamental frequency, the duration of the sounds and their energy. Any error in estimating these parameters may lead to a wrong decision. MULTISPEECH will investigate estimating the uncertainty of the duration of the phones (see uncertainty of phonetic boundaries above) and on the fundamental frequency, as well as how this uncertainty shall be propagated in the detection of prosodic phenomena such as accented words, utterance modality, or determination of the structure of the utterance.

ORPAILLEUR Project-Team

3. Research Program

3.1. Knowledge Discovery guided by Domain Knowledge

Keywords: knowledge discovery in databases, knowledge discovery in databases guided by domain knowledge, data mining formal concept analysis, classification, pattern mining second-order Hidden Markov Models

Knowledge discovery in databases (KDD) is aimed at discovering patterns in large databases. These patterns can then be interpreted as knowledge units to be reused in knowledge systems. From an operational point of view, the KDD process is based on three main steps: (i) selection and preparation of the data, (ii) data mining, (iii) interpretation of the discovered patterns. The KDD process –as implemented in the Orpailleur team– is based on data mining methods which are either symbolic or numerical. Symbolic methods are based on pattern mining (e.g. mining frequent itemsets, association rules, sequences...), Formal Concept Analysis (FCA [80]) and extensions of FCA such as Pattern Structures [83] and Relational Concept Analysis (RCA [90]). Numerical methods are based on probabilistic approaches such as second-order Hidden Markov Models (HMM [85]), which are well adapted to the mining of temporal and spatial data.

Domain knowledge, when available, can improve and guide the KDD process, materializing the idea of *Knowledge Discovery guided by Domain Knowledge* or KDDK. In KDDK, domain knowledge plays a role at each step of KDD: the discovered patterns can be interpreted as knowledge units and reused for problem-solving activities in knowledge systems, implementing the operational sequence "mining, interpreting (modeling), representing, and reasoning". In this way, knowledge discovery appears as a core task in knowledge engineering, with an impact in various semantic activities, e.g. information retrieval, recommendation and ontology engineering. Usual application domains for the team include agronomy, astronomy, biology, chemistry, and medicine.

One main operation in the research work of Orpailleur on KDDK is *classification*, which is a polymorphic process involved in modeling, mining, representing, and reasoning tasks. Classification problems can be formalized by means of a class of objects (or individuals), a class of attributes (or properties), and a binary correspondence between the two classes, indicating for each individual-property pair whether the property applies to the individual or not. The properties may be features that are present or absent, or the values of a property that have been transformed into binary variables. Formal Concept Analysis (FCA) relies on the analysis of such binary tables and may be considered as a symbolic data mining technique to be used for extracting a set of formal concepts then organized within a concept lattice [80] (concept lattices are also known as "Galois lattices" [68]).

In parallel, the search for frequent itemsets and the extraction of association rules are well-known symbolic data mining methods, related to FCA (actually searching for frequent itemsets can be understood as traversing a concept lattice). Both processes usually produce a large number of items and rules, leading to the associated problems of "mining the sets of extracted items and rules". Some subsets of itemsets, e.g. frequent closed itemsets (FCIs), allow finding interesting subsets of association rules, e.g. informative association rules. This explains why several algorithms are needed for mining data depending on specific applications [92].

3.2. Text Mining

Keywords: text mining, knowledge discovery form collection of texts, annotation, ontology engineering from texts

The objective of a text mining process is to extract useful knowledge units from large collections of texts [78]. The text mining process shows specific characteristics due to the fact that texts are complex objects written in natural language. The information in a text is expressed in an informal way, following linguistic rules, making text mining a particular task. To avoid information dispersion, a text mining process has to take into account –as much as possible– paraphrases, ambiguities, specialized vocabulary and terminology. This is why the preparation of texts for text mining is usually dependent on linguistic resources and methods.

From a KDDK perspective, text mining is aimed at extracting "interesting units" (nouns and relations) from texts with the help of domain knowledge encoded within an ontology (also useful for text annotation). Text mining is especially useful in the context of semantic web for ontology engineering. In the Orpailleur team, the focus is put on the mining of real-world texts in application domains such as biology and medicine, using mainly symbolic data mining methods, and especially Formal Concept Analysis. Accordingly, the text mining process may be involved in a loop used to enrich and to extend linguistic resources. In turn, linguistic and ontological resources can be exploited to guide a "knowledge-based text mining process".

3.3. Knowledge Systems and Web of Data

Keywords: knowledge engineering, web of data, semantic web, ontology, description logics, classification-based reasoning, case-based reasoning, information retrieval

The web of data constitutes a good platform for experimenting ideas on knowledge engineering and knowledge discovery, in relation with the principles of semantic web. A software agent may be able to read, understand, and manipulate information on the web, if and only if the knowledge necessary for achieving those tasks is available: this is why domain knowledge and ontologies are of main importance. The knowledge representation language recommended by W3C to design ontologies and knowledge bases is OWL, which is based on description logics (DLs [65]). In OWL, knowledge units are represented by classes (DL concepts) having properties (DL roles) and instances. Concepts are organized within a partial order based on a subsumption relation, and the inference services are based on classification-based reasoning and case-based reasoning (CBR).

Actually, there are many interconnections between concept lattices in FCA and ontologies, e.g. the partial order underlying an ontology can be supported by a concept lattice. Moreover, a pair of implications within a concept lattice can be adapted for designing concept definitions in ontologies. Accordingly, we are interested here in two main challenges: how the web of data, as a set of potential knowledge sources (e.g. DBpedia, Wikipedia, Yago, Freebase...) can be mined for helping the design of definitions and knowledge bases and how knowledge discovery techniques can be applied for providing a better usage of the web of data (e.g. LOD classification).

Accordingly, a part of the research work in Knowledge Engineering is oriented towards knowledge discovery in the web of data, as, with the increased interest in machine processable data, more and more data is now published in RDF (Resource Description Framework) format. Particularly, we are interested in the completeness of the data and their potential to provide concept definitions in terms of necessary and sufficient conditions [66]. We have proposed a novel technique based on FCA which allows data exploration as well as the discovery of definition (bidirectional implication rules).

PANAMA Project-Team

3. Research Program

3.1. Axis 1: Sparse Models and Representations

3.1.1. Efficient Sparse Models and Dictionary Design for Large-scale Data

Sparse models are at the core of many research domains where the large amount and high-dimensionality of digital data requires concise data descriptions for efficient information processing. Recent breakthroughs have demonstrated the ability of these models to provide concise descriptions of complex data collections, together with algorithms of provable performance and bounded complexity.

A crucial prerequisite for the success of today's methods is the knowledge of a "dictionary" characterizing how to concisely describe the data of interest. Choosing a dictionary is currently something of an "art", relying on expert knowledge and heuristics.

Pre-chosen dictionaries such as wavelets, curvelets or Gabor dictionaries, are based upon stylized signal models and benefit from fast transform algorithms, but they fail to fully describe the content of natural signals and their variability. They do not address the huge diversity underlying modern data much beyond time series and images: data defined on graphs (social networks, internet routing, brain connectivity), vector valued data (diffusion tensor imaging of the brain), multichannel or multi-stream data (audiovisual streams, surveillance networks, multimodal biomedical monitoring).

The alternative to a pre-chosen dictionary is a trained dictionary learned from signal instances. While such representations exhibit good performance on small-scale problems, they are currently limited to low-dimensional signal processing due to the necessary training data, memory requirements and computational complexity. Whether designed or learned from a training corpus, dictionary-based sparse models and the associated methodology fail to scale up to the volume and resolution of modern digital data, for they intrinsically involve difficult linear inverse problems. To overcome this bottleneck, a new generation of efficient sparse models is needed, beyond dictionaries, encompassing the ability to provide sparse and structured data representations as well as computational efficiency. For example, while dictionaries describe low-dimensional signal models in terms of their "synthesis" using few elementary building blocks called atoms, in "analysis" alternatives the low-dimensional structure of the signal is rather "carved out" by a set of equations satisfied by the signal. Linear as well as nonlinear models can be envisioned.

3.1.2. Compressive Learning

A flagship emerging application of sparsity is the paradigm of compressive sensing, which exploits sparse models at the analog and digital levels for the acquisition, compression and transmission of data using limited resources (fewer/less expensive sensors, limited energy consumption and transmission bandwidth, etc.). Besides sparsity, a key pillar of compressive sensing is the use of random low-dimensional projections. Through compressive sensing, random projections have shown their potential to allow drastic dimension reduction with controlled information loss, provided that the projected signal vector admits a sparse representation in some transformed domain. A related scientific domain, where sparsity has been recognized as a key enabling factor, is Machine Learning, where the overall goal is to design statistically founded principles and efficient algorithms in order to infer general properties of large data collections through the observation of a limited number of representative examples. Marrying sparsity and random low-dimensional projections with machine learning shall allow the development of techniques able to efficiently capture and process the information content of large data collections. The expected outcome is a dramatic increase of the impact of sparse models in machine learning, as well as an integrated framework from the signal level (signals and their acquisition) to the semantic level (information and its manipulation), and applications to data sizes and volumes of collections that cannot be handled by current technologies.

3.2. Axis 2: Robust Acoustic Scene Analysis

3.2.1. Compressive Acquisition and Processing of Acoustic Scenes

Acoustic imaging and scene analysis involve acquiring the information content from acoustic fields with a limited number of acoustic sensors. A full 3D+t field at CD quality and Nyquist spatial sampling represents roughly 10^6 microphones/m^3. Dealing with such high-dimensional data requires to drastically reduce the data flow by positioning appropriate sensors, and selecting from all spatial locations the few spots where acoustic sources are active. The main goal is to develop a theoretical and practical understanding of the conditions under which compressive acoustic sensing is both feasible and robust to inaccurate modeling, noisy measures, and partially failing or uncalibrated sensing devices, in various acoustic sensing scenarii. This requires the development of adequate algorithmic tools, numerical simulations, and experimental data in simple settings where hardware prototypes can be implemented.

3.2.2. Robust Audio Source Separation

Audio signal separation consists in extracting the individual sound of different instruments or speakers that were mixed on a recording. It is now successfully addressed in the academic setting of linear instantaneous mixtures. Yet, real-life recordings, generally associated to reverberant environments, remain an unsolved difficult challenge, especially with many sources and few audio channels. Much of the difficulty comes from the combination of (i) complex source characteristics, (ii) sophisticated underlying mixing model and (iii) adverse recording environments. Moreover, as opposed to the “academic” blind source separation task, most applicative contexts and new interaction paradigms offer a variety of situations in which prior knowledge and adequate interfaces enable the design and the use of informed and/or manually assisted source separation methods.

The former METISS team has developed a generic and flexible probabilistic audio source separation framework that has the ability to combine various acoustic models such as spatial and spectral source models. Building on this existing framework, a first objective of PANAMA is to instantiate and validate specific instances of this framework targeted to real-world industrial applications, such as 5.1 movie re-mastering, interactive music soloist control and outdoor speech enhancement. Extensions of the framework are needed to achieve real-time online processing, and advanced constraints or probabilistic priors for the sources at hand need to be designed, while paying attention to computational scalability issues.

In parallel to these efforts, expected progress in sparse modeling for inverse problems shall bring new approaches to source separation and modeling, as well as to source localization, which is often an important first step in a source separation workflow.

3.2.3. Robust Audio Source Localization

Audio source localization consists in estimating the position of one or several sound sources given the signals received by a microphone array. Knowing the geometry of an audio scene is often a pre-requisite to perform higher-level tasks such as speaker identification and tracking, speech enhancement and recognition or audio source separation. It can be decomposed into two sub-tasks : (i) compute spatial auditory features from raw audio input and (ii) map these features to the desired spatial information. Robustly addressing both these aspects with a limited number of microphones, in the presence of noise, reverberation, multiple and possibly moving sources remains a key challenge in audio signal processing. The first aspect will be tackled by both advanced statistical and acoustical modeling of spatial auditory features. The second one will be addressed by two complementary approaches. *Physics-driven* approaches cast sound source localization as an inverse problem given the known physics of sound propagation within the considered system. *Data-driven* approaches aim at learning the desired feature-to-source-position mapping using real-world or synthetic training datasets adapted to the problem at hand. Combining these approaches should allow a widening of the notion of source localization, considering problems such as the identification of the directivity or diffuseness of the source as well as some of the boundary conditions of the room. A general perspective is to investigate the relations between the physical structure of the source and the particular structures that can be discovered or enforced in the representations and models used for characterization, localization and separation.

3.3. Axis 3: Large-scale Audio Content Processing and Self-organization

3.3.1. Motif Discovery in Audio Data

Facing the ever-growing quantity of multimedia content, the topic of motif discovery and mining has become an emerging trend in multimedia data processing with the ultimate goal of developing weakly supervised paradigms for content-based analysis and indexing. In this context, speech, audio and music content, offers a particularly relevant information stream from which meaningful information can be extracted to create some form of "audio icons" (key-sounds, jingles, recurrent locutions, musical choruses, etc ...) without resorting to comprehensive inventories of expected patterns.

This challenge raises several fundamental questions that will be among our core preoccupations over the next few years. The first question is the deployment of motif discovery on a large scale, a task that requires extending audio motif discovery approaches to incorporate efficient time series pattern matching methods (fingerprinting, similarity search indexing algorithms, stochastic modeling, etc.). The second question is that of the use and interpretation of the motifs discovered. Linking motif discovery and symbolic learning techniques, exploiting motif discovery in machine learning are key research directions to enable the interpretation of recurring motifs.

On the application side, several use cases can be envisioned which will benefit from motif discovery deployed on a large scale. For example, in spoken content, word-like repeating fragments can be used for several spoken document-processing tasks such as language-independent topic segmentation or summarization. Recurring motifs can also be used for audio summarization of audio content. More fundamentally, motif discovery paves the way for a shift from supervised learning approaches for content description to unsupervised paradigms where concepts emerge from the data.

3.3.2. Structure Modeling and Inference in Audio and Musical Contents

Structuring information is a key step for the efficient description and learning of all types of contents, and in particular audio and musical contents. Indeed, structure modeling and inference can be understood as the task of detecting dependencies (and thus establishing relationships) between different fragments, parts or sections of information content.

A stake of structure modeling is to enable more robust descriptions of the properties of the content and better model generalization abilities that can be inferred from a particular content, for instance via cache models, trigger models or more general graphical models designed to render the information gained from structural inference. Moreover, the structure itself can become a robust descriptor of the content, which is likely to be more resistant than surface information to a number of operations such as transmission, transduction, copyright infringement or illegal use.

In this context, information theory concepts need to be investigated to provide criteria and paradigms for detecting and modeling structural properties of audio contents, covering potentially a wide range of application domains in speech content mining, music modeling or audio scene monitoring.

PERCEPTION Project-Team

3. Research Program

3.1. Audio-Visual Scene Analysis

From 2006 to 2009, R. Horaud was the scientific coordinator of the collaborative European project POP (Perception on Purpose), an interdisciplinary effort to understand visual and auditory perception at the crossroads of several disciplines (computational and biological vision, computational auditory analysis, robotics, and psychophysics). This allowed the PERCEPTION team to launch an interdisciplinary research agenda that has been very active for the last five years. There are very few teams in the world that gather scientific competences spanning computer vision, audio signal processing, machine learning and human-robot interaction. The fusion of several sensorial modalities resides at the heart of the most recent biological theories of perception. Nevertheless, multi-sensor processing is still poorly understood from a computational point of view. In particular and so far, audio-visual fusion has been investigated in the framework of speech processing using close-distance cameras and microphones. The vast majority of these approaches attempt to model the temporal correlation between the auditory signals and the dynamics of lip and facial movements. Our original contribution has been to consider that audio-visual localization and recognition are equally important. We have proposed to take into account the fact that the audio-visual objects of interest live in a three-dimensional physical space and hence we contributed to the emergence of *audio-visual scene analysis* as a scientific topic in its own right. We proposed several novel statistical approaches based on supervised and unsupervised mixture models. The *conjugate mixture model* (CMM) is an unsupervised probabilistic model that allows to cluster observations from different modalities (e.g., vision and audio) living in different mathematical spaces [18], [2]. We thoroughly investigated CMM, provided practical resolution algorithms and studied their convergence properties. We developed several methods for sound localization using two or more microphones [1]. The *Gaussian locally-linear model* (GLLiM) is a partially supervised mixture model that allows to map high-dimensional observations (audio, visual, or concatenations of audio-visual vectors) onto low-dimensional manifolds with a partially known structure [6]. This model is particularly well suited for perception because it encodes both observable and unobservable phenomena. A variant of this model, namely *probabilistic piecewise affine mapping* has also been proposed and successfully applied to the problem of sound-source localization and separation [5]. The European projects HUMAVIPS (2010-2013) coordinated by R. Horaud and EARS (2014-2017), applied audio-visual scene analysis to human-robot interaction.

3.2. Stereoscopic Vision

Stereoscopy is one of the most studied topics in biological and computer vision. Nevertheless, classical approaches of addressing this problem fail to integrate eye/camera vergence. From a geometric point of view, the integration of vergence is difficult because one has to re-estimate the epipolar geometry at every new eye/camera rotation. From an algorithmic point of view, it is not clear how to combine depth maps obtained with different eyes/cameras relative orientations. Therefore, we addressed the more general problem of binocular vision that combines the low-level eye/camera geometry, sensor rotations, and practical algorithms based on global optimization [12], [20]. We studied the link between mathematical and computational approaches to stereo (global optimization and Markov random fields) and the brain plausibility of some of these approaches: indeed, we proposed an original mathematical model for the complex cells in visual-cortex areas V1 and V2 that is based on steering Gaussian filters and that admits simple solutions [13]. This addresses the fundamental issue of how local image structure is represented in the brain/computer and how this structure is used for estimating a dense disparity field. Therefore, the main originality of our work is to address both computational and biological issues within a unifying model of binocular vision. Another equally important problem that still remains to be solved is how to integrate binocular depth maps over time. Recently, we have addressed this problem and proposed a semi-global optimization framework that starts with sparse yet reliable matches and proceeds with propagating them over both space and time. The concept of seed-match propagation has then been extended to TOF-stereo fusion [8].

3.3. Audio Signal Processing

Audio-visual fusion algorithms necessitate that the two modalities are represented in the same mathematical space. Binaural audition allows to extract sound-source localization (SSL) information from the acoustic signals recorded with two microphones. We have developed several methods, that perform sound localization in the temporal and the spectral domains. If a direct path is assumed, one can exploit the *time difference of arrival* (TDOA) between two microphones to recover the position of the sound source with respect to the position of the two microphones. The solution is not unique in this case, the sound source lies onto a 2D manifold. However, if one further assumes that the sound source lies in a horizontal plane, it is then possible to extract the azimuth. We used this approach to predict possible sound locations in order to estimate the direction of a speaker [2]. We also developed a geometric formulation and we showed that with four non-coplanar microphones the azimuth and elevation of a single source can be estimated without ambiguity [1]. We also investigated SSL in the spectral domain. This exploits the filtering effects of the head related transfer function (HRTF): there is a different HRTF for the left and right microphones. The interaural spectral features, namely the ILD (interaural level difference) and IPD (interaural phase difference) can be extracted from the short-time Fourier transforms of the two signals. The sound direction is encoded in these interaural features but it is not clear how to make SSL explicit in this case. We proposed a supervised learning formulation that estimates a mapping from interaural spectral features (ILD and IPD) to source directions using two different setups: audio-motor learning [5] and audio-visual learning [7].

3.4. Visual Reconstruction With Multiple Color and Depth Cameras

For the last decade, one of the most active topics in computer vision has been the visual reconstruction of objects, people, and complex scenes using a multiple-camera setup. The PERCEPTION team has pioneered this field and by 2006 several team members published seminal papers in the field. Recent work has concentrated onto the robustness of the 3D reconstructed data using probabilistic outlier rejection techniques combined with algebraic geometry principles and linear algebra solvers [23]. Subsequently, we proposed to combine 3D representations of shape (meshes) with photometric data [21]. The originality of this work was to represent photometric information as a scalar function over a discrete Riemannian manifold, thus *generalizing image analysis to mesh and graph analysis*. Manifold equivalents of local-structure detectors and descriptors were developed [22]. The outcome of this pioneering work has been twofold: the formulation of a new research topic now addressed by several teams in the world, and allowed us to start a three year collaboration with Samsung Electronics. We developed the novel concept of *mixed camera systems* combining high-resolution color cameras with low-resolution depth cameras [14], [10],[9]. Together with our start-up company 4D Views Solutions and with Samsung, we developed the first practical depth-color multiple-camera multiple-PC system and the first algorithms to reconstruct high-quality 3D content [8].

3.5. Registration, Tracking and Recognition of People and Actions

The analysis of articulated shapes has challenged standard computer vision algorithms for a long time. There are two difficulties associated with this problem, namely how to represent articulated shapes and how to devise robust registration and tracking methods. We addressed both these difficulties and we proposed a novel kinematic representation that integrates concepts from robotics and from the geometry of vision. In 2008 we proposed a method that parameterizes the occluding contours of a shape with its intrinsic kinematic parameters, such that there is a direct mapping between observed image features and joint parameters [19]. This deterministic model has been motivated by the use of 3D data gathered with multiple cameras. However, this method was not robust to various data flaws and could not achieve state-of-the-art results on standard dataset. Subsequently, we addressed the problem using probabilistic generative models. We formulated the problem of articulated-pose estimation as a maximum-likelihood with missing data and we devised several tractable algorithms [17], [16]. We proposed several expectation-maximization procedures applied to various articulated shapes: human bodies, hands, etc. In parallel, we proposed to segment and register articulated shapes represented with graphs by embedding these graphs using the spectral properties of graph Laplacians [4]. This turned out to be a very original approach that has been followed by many other researchers in computer vision and computer graphics.

PERVASIVE INTERACTION Team

3. Research Program

3.1. Situation Models

Situation Modelling, Situation Awareness, Probabilistic Description Logistics

The objectives of this research area are to develop and refine new computational techniques that improve the reliability and performance of situation models, extend the range of possible application domains, and reduce the cost of developing and maintaining situation models. Important research challenges include developing machine-learning techniques to automatically acquire and adapt situation models through interaction, development of techniques to reason and learn about appropriate behaviors, and the development of new algorithms and data structures for representing situation models.

Over the next four years we will address the following research challenges:

Techniques for learning and adapting situation models: Hand crafting of situation models is currently an expensive process requiring extensive trial and error. We will investigate combination of interactive design tools coupled with supervised and semi-supervised learning techniques for constructing initial, simplified prototype situation models in the laboratory. One possible approach is to explore developmental learning to enrich and adapt the range of situations and behaviors through interaction with users.

Reasoning about actions and behaviors: Constructing systems for reasoning about actions and their consequences is an important open challenge. We will explore integration of planning techniques for operationalizing actions sequences within behaviors, and for constructing new action sequences when faced with unexpected difficulties. We will also investigate reasoning techniques within the situation modeling process for anticipating the consequences of actions, events and phenomena.

Algorithms and data structures for situation models: In recent years, we have experimented with an architecture for situated interaction inspired by work in human factors. This model organises perception and interaction as a cyclic process in which directed perception is used to detect and track entities, verify relations between entities, detect trends, anticipate consequences and plan actions. Each phase of this process raises interesting challenges questions algorithms and programming techniques. We will experiment alternative programming techniques representing and reasoning about situation models both in terms of difficulty of specification and development and in terms of efficiency of the resulting implementation. We will also investigate the use of probabilistic graph models as a means to better accommodate uncertain and unreliable information. In particular, we will experiment with using probabilistic predicates for defining situations, and maintaining likelihood scores over multiple situations within a context. Finally, we will investigate the use of simulation as technique for reasoning about consequences of actions and phenomena.

Probabilistic Description Logics: In our work, we will explore the use of probabilistic predicates for representing relations within situation models. As with our earlier work, entities and roles will be recognized using multi-modal perceptual processes constructed with supervised and semi-supervised learning [Brdiczka 07], [Barraquand 12]. However, relations will be expressed with probabilistic predicates. We will explore learning based techniques to probabilistic values for elementary predicates, and propagate these through probabilistic representation for axioms using Probabilistic Graphical Models and/or Bayesian Networks.

The challenges in this research area will be addressed through three specific research actions covering situation modelling in homes, learning on mobile devices, and reasoning in critical situations.

3.1.1. Learning Routine patterns of activity in the home.

The objective of this research action is to develop a scalable approach to learning routine patterns of activity in a home using situation models. Information about user actions is used to construct situation models in which key elements are semantic time, place, social role and actions. Activities are encoded as sequences of situations. Recurrent activities are detected as sequences of activities that occur at a specific time and place each day. Recurrent activities provide routines what can be used to predict future actions and anticipate needs and services. An early demonstration has been to construct an intelligent assistant that can respond to and filter communications.

This research action is carried out as part of the doctoral research of Julian Cumin in cooperation with researchers at Orange labs, Meylan. Results are to be published at Ubicomp, Ambient intelligence, Intelligent Environments and IEEE Transactions on System Man and Cybernetics. Julien Cumin will complete and defend his doctoral thesis in 2018.

3.1.2. Learning Patterns of Activity with Mobile Devices

The objective of this research action is to develop techniques to observe and learn recurrent patterns of activity using the full suite of sensors available on mobile devices such as tablets and smart phones. Most mobile devices include seven or more sensors organized in 4 groups: Positioning Sensors, Environmental Sensors, Communications Subsystems, and Sensors for Human-Computer Interaction. Taken together, these sensors can provide a very rich source of information about individual activity.

In this area we explore techniques to observe activity with mobiles devices in order to learn daily patterns of activity. We will explore supervised and semi-supervised learning to construct systems to recognize places and relevant activities. Location and place information, semantic time of day, communication activities, inter-personal interactions, and travel activities (walking, driving, riding public transportation, etc.) are recognized as probabilistic predicates and used to construct situation models. Recurrent sequences of situations will be detected and recorded to provide an ability to predict upcoming situations and anticipate needs for information and services.

Our goal is to develop a theory for building context aware services that can be deployed as part of the mobile applications that companies such as SNCF and RATP use to interact with clients. For example, a current project concerns systems that observe daily travel routines for the Paris region RATP metro and SNCF commuter trains. This system learns individual travel routines on the mobile device without the need to divulge information about personal travel to a cloud based system. The resulting service will consult train and metro schedules to assure that planned travel is feasible and to suggest alternatives in the case of travel disruptions. Similar applications are under discussion for the SNCF inter-city travel and Air France for air travel.

This research action is conducted in collaboration with the Inria Startup Situ8ed. The current objective is to deploy and evaluate a first prototype App during 2017. Techniques will be used commercially by Situ8ed for products to be deployed as early as 2019.

3.1.3. Observing and Modelling Competence and Awareness in Critical Situations

The aim of this research action is to experimentally evaluate and compare current theories for mental modelling for problem solving and attention in stressful situations, as well as to refine theories and techniques for observing visual fixation, attention and emotion. We are currently investigating differences in visual attention, emotional response and mental states of chess experts and chess novices solving chess problems and participating in chess matches. We observe physiological responses, mental states and visual attention using eye-tracking, long term and instantaneous face-expressions (micro-expressions), skin conductivity, blood flow (BVP), posture and other information extracted from audio-visual recordings of players.

We expect that a high degree of expertise in chess should be reflected in patterns of eye movement and emotional reaction in accordance with the game situation. Information from visual attention will be used to determine and model the degree to which a player understands the game situation in terms of abstract configurations of chess pieces rather than the positions of individual pieces. Information about the emotional reactions of players will be expressed as trajectories in the physiological space of pleasure, arousal and dominance to determine if a players understanding of the game situation can be observed from emotional reaction to game play.

This work is supported by the ANR project CEEGE in cooperation with the department of NeuroCognition of Univ. Bielefeld, as well as the LIG internal project AirBorne in cooperation with the French Air Force training center at ISTRE. Work in this area includes the Doctoral research of Thomas Guntz to be defended in 2019.

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3.2. Perception of People, Activities and Emotions

Machine perception is fundamental for situated behavior. Work in this area will concern construction of perceptual components using computer vision, acoustic perception, accelerometers and other embedded sensors. These include low-cost accelerometers [Bao 04], gyroscopic sensors and magnetometers, vibration sensors, electromagnetic spectrum and signal strength (wifi, bluetooth, GSM), infrared presence detectors, and bolometric imagers, as well as microphones and cameras. With electrical usage monitoring, every power switch can be used as a sensor [Fogarty 06], [Coutaz 16]. We will develop perceptual components for integrated vision systems that combine a low-cost imaging sensors with on-board image processing and wireless communications in a small, low-cost package. Such devices are increasingly available, with the enabling manufacturing technologies driven by the market for integrated imaging sensors on mobile devices. Such technology enables the use of embedded computer vision as a practical sensor for smart objects.

Research challenges to be addressed in this area include development of practical techniques that can be deployed on smart objects for perception of people and their activities in real world environments, integration and fusion of information from a variety of sensor modalities with different response times and levels of abstraction, and perception of human attention, engagement, and emotion using visual and acoustic sensors.

Work in this research area will focus on three specific Research Actions

3.2.1. Multi-modal perception and modeling of activities

The objective of this research action is to develop techniques for observing and scripting activities for common household tasks such as cooking and cleaning. An important part of this project involves acquiring annotated multi-modal datasets of activity using an extensive suite of visual, acoustic and other sensors. We are interested in real-time on-line techniques that capture and model full body movements, head motion and manipulation actions as 3D articulated motion sequences decorated with semantic labels for individual actions and activities with multiple RGB and RGB-D cameras.

We will explore the integration of 3D articulated models with appearance based recognition approaches and statistical learning for modeling behaviors. Such techniques provide an important enabling technology for context aware services in smart environments [Coutaz 05], [Crowley 15], investigated by Pervasive Interaction team, as well as research on automatic cinematography and film editing investigated by the Imagine team [Gandhi 13] [Gandhi 14] [Ronfard 14] [Galvane 15]. An important challenge is to determine which techniques are most appropriate for detecting, modeling and recognizing a large vocabulary of actions and activities under different observational conditions.

We will explore representations of behavior that encodes both temporal-spatial structure and motion at multiple levels of abstraction. We will further propose parameters to encode temporal constraints between actions in the activity classification model using a combination of higher-level action grammars [Pirsiavash 14] and episodic reasoning [Santofimia 14] [Edwards 14].

Our method will be evaluated using long-term recorded dataset that contains recordings of activities in home environments. This work will be reported in the IEEE Conference on Face and Gesture Recognition, IEEE transactions on Pattern Analysis and Machine Intelligence, (PAMI) et IEEE Transactions on Systems man and Cybernetics. This work is carried out in the doctoral research of Nachwa Abubakr in cooperation with Remi Ronfard of the Imagine Team of Inria.

3.2.2. Perception with low-cost integrated sensors

In this research action, we will continue work on low-cost integrated sensors using visible light, infrared, and acoustic perception. We will continue development of integrated visual sensors that combine micro-cameras and embedded image processing for detecting and recognizing objects in storage areas. We will combine visual and acoustic sensors to monitor activity at work-surfaces. Low cost real-time image analysis procedures will be designed that acquire and process images directly as they are acquired by the sensor.

Bolometric image sensors measure the Far Infrared emissions of surfaces in order to provide an image in which each pixel is an estimate of surface temperature. Within the European MIRTIC project, Grenoble startup, ULIS has created a relatively low-cost Bolometric image sensor (Retina) that provides small images of 80 by 80 pixels taken from the Far-infrared spectrum. Each pixel provides an estimate of surface temperature. Working with Schneider Electric, engineers in the Pervasive Interaction team had developed a small, integrated sensor that combines the MIRTIC Bolometric imager with a microprocessor for on-board image processing. The package has been equipped with a fish-eye lens so that an overhead sensor mounted at a height of 3 meters has a field of view of approximately 5 by 5 meters. Real-time algorithms have been demonstrated for detecting, tracking and counting people, estimating their trajectories and work areas, and estimating posture.

Many of the applications scenarios for Bolometric sensors proposed by Schneider Electric assume a scene model that assigns pixels to surfaces of the floor, walls, windows, desks or other items of furniture. The high cost of providing such models for each installation of the sensor would prohibit most practical applications. We have recently developed a novel automatic calibration algorithm that determines the nature of the surface under each pixel of the sensor.

Work in this area will continue to develop low-cost real time infrared image sensing, as well as explore combinations of far-infrared images with RGB and RGBD images.

3.2.3. Observation of emotion from physiological responses in critical situations

Recent research in Cognitive Science indicates that the human emotions result in physiological manifestations in the heart rate, skin conductance, skin color, body movements and facial expressions. It has been proposed that these manifestations can be measured by observation of skin color, body motions, and facial expressions and modeled as activation levels in three dimensions known as Valence, Arousal and Dominance. The goal if this project is to evaluate the effectiveness of visual and acoustic perception technique for measuring these physiological manifestations.

Experimental data will be collected by observing subjects engaged in playing chess. A special apparatus has been constructed that allows synchronized recording from a color camera, Kinect2 3D camera, and Tobi Eye Tracker of a player seated before a computer generated display of a chess board. The masters student will participate in the definition and recording of scenarios for recording test data, apply recently proposed techniques from the scientific literature for measuring emotions, and provide a comparative performance evaluation of various techniques. The project is expected to reveal the relative effectiveness of computer vision and other techniques for observing human emotions.

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3.3. Sociable Interaction with Smart Objects

Reeves and Nass argue that a social interface may be the truly universal interface [Reeves 98]. Current systems lack ability for social interaction because they are unable to perceive and understand humans or to learn from interaction with humans. One of the goals of the research to be performed in Pervasive Interaction is to provide such abilities.

Work in research area RA3 will demonstrate the use of situation models for sociable interaction with smart objects and companion robots. We will explore the use of situation models as a representation for sociable interaction. Our goal in this research is to develop methods to endow an artificial agent with the ability to acquire social common sense using the implicit feedback obtained from interaction with people. We believe that such methods can provide a foundation for socially polite man-machine interaction, and ultimately for other forms of cognitive abilities. We propose to capture social common sense by training the appropriateness of behaviors in social situations. A key challenge is to employ an adequate representation for social situations.

Knowledge for sociable interaction will be encoded as a network of situations that capture both linguistic and non-verbal interaction cues and proper behavioral responses. Stereotypical social interactions will be represented as trajectories through the situation graph. We will explore methods that start from simple stereotypical situation models and extending a situation graph through the addition of new situations and the splitting of existing situations. An important aspect of social common sense is the ability to act appropriately in social situations. We propose to learn the association between behaviors and social situation using reinforcement learning. Situation models will be used as a structure for learning appropriateness of actions and behaviors that may be chosen in each situation, using reinforcement learning to determine a score for appropriateness based on feedback obtained by observing partners during interaction.

Work in this research area will focus on four specific Research Actions

3.3.1. *Moving with people*

Our objective in this area is to establish the foundations for robot motions that are aware of human social situation that move in a manner that complies with the social context, social expectations, social conventions and cognitive abilities of humans. Appropriate and socially compliant interactions require the ability for real time perception of the identity, social role, actions, activities and intents of humans. Such perception can be used to dynamically model the current situation in order to understand the situation and to compute the appropriate course of action for the robot depending on the task at hand.

To reach this objective, we propose to investigate three interacting research areas:

- Modeling the context and situation of human activities for motion planning
- Planning and acting in a social context.
- Identifying and modeling interaction behaviors.

In particular, we will investigate techniques that allow a tele-presence robot, such as the BEAM system, to autonomously navigate in crowds of people as may be found at the entry to a conference room, or in the hallway of a scientific meeting. We will also continue experiments on autonomous motion for personal assistance robots (project PRAMAD). Work in this area includes the doctoral work of Jos,aö¬© da Silva, to be defended in 2019.

3.3.2. Understanding and communicating intentions from motion

This research area concerns the communication through motion. When two or more people move as a group, their motion is regulated by implicit rules that signal a shared sense of social conventions and social roles. For example, moving towards someone while looking directly at them signals an intention for engagement. In certain cultures, subtle rules dictate who passes through a door first or last. When humans move in groups, they implicitly communicate intentions with motion. In this research area, we will explore the scientific literature on proxemics and the social sciences on such movements, in order to encode and evaluate techniques for socially appropriate motion by robots.

3.3.3. Socially aware interaction

This research area concerns socially aware man-machine interaction. Appropriate and socially compliant interaction requires the ability for real time perception of the identity, social role, actions, activities and intents of humans. Such perception can be used to dynamically model the current situation in order to understand the context and to compute the appropriate course of action for the task at hand. Performing such interactions in manner that respects and complies with human social norms and conventions requires models for social roles and norms of behavior as well as the ability to adapt to local social conventions and individual user preferences. In this research area, we will complement research area 3.2 with other forms of communication and interaction, including expression with stylistic face expressions rendered on a tablet, facial gestures, body motions and speech synthesis. We will experiment with use of commercially available tool for spoken language interaction in conjunction with expressive gestures.

3.3.4. Stimulating affection and persuasion with affective devices.

This research area concerns technologies that can stimulate affection and engagement, as well as induce changes in behavior. When acting as a coach or cooking advisor, smart objects must be credible and persuasive. One way to achieve this goal is to express affective feedbacks while interacting. This can be done using sound, light and/or complex moves when the system is composed of actuators.

Research in this area will address 3 questions:

1. How do human perceive affective signals expressed by smart objects (including robots)?
2. How does physical embodiment effect perception of affect by humans?
3. What are the most effective models and tools for animation of affective expression?

Both the physical form and the range of motion have important impact on the ability of a system to inspire affection. We will create new models to propose a generic animation model, and explore the effectiveness of different forms of motion in stimulating affect.

3.3.5. Bibliography

[Reeves 98] B. Reeves and C. Nass, The Media Equation: how People Treat Computers, Television, and New Media Like Real People and Places. Cambridge University Press, 1998.

3.4. Interaction with Pervasive Smart Objects and Displays

Currently, the most effective technologies for new media for sensing, perception and experience are provided by virtual and augmented realities [Van Krevelen 2010]. At the same time, the most effective means to augment human cognitive abilities are provided by access to information spaces such as the world-wide-web using graphical user interfaces. A current challenge is to bring these two media together.

Display technologies continue to decrease exponentially, driven largely by investment in consumer electronics as well as the overall decrease in cost of microelectronics. A consequence has been an increasing deployment of digital displays in both public and private spaces. This trend is likely to accelerate, as new technologies and growth in available communications bandwidth enable ubiquitous low-cost access to information and communications.

The arrival of pervasive displays raises a number of interesting challenges for situated multi-modal interaction. For example:

1. Can we use perception to detect user engagement and identify users in public spaces?
2. Can we replace traditional pointing hardware with gaze and gesture based interaction?
3. Can we tailor information and interaction for truly situated interaction, providing the right information at the right time using the right interaction modality?
4. How can we avoid information overload and unnecessary distraction with pervasive displays?

It is increasingly possible to embed sensors and displays in clothing and ordinary devices, leading to new forms of tangible and wearable interaction with information. This raises challenges such as

1. What are the tradeoffs between large-scale environmental displays and wearable displays using technologies such as e-textiles and pico-projector?
2. How can we manage the tradeoffs between implicit and explicit interaction with both tangible and wearable interaction?
3. How can we determine the appropriate modalities for interaction?
4. How can we make users aware of interaction possibilities without creating distraction?

In addition to display and communications, the continued decrease in microelectronics has also driven an exponential decrease in cost of sensors, actuators, and computing resulting in an exponential growth in the number of smart objects in human environments. Current models for systems organization are based on centralized control, in which a controller or local hub, orchestrates smart objects, generally in connection with cloud computing. This model creates problems with privacy and ownership of information. An alternative is to organize local collections of smart objects to provide distributed services without the use of a centralized controller. The science of ecology can provide an architectural model for such organization.

This approach raises a number of interesting research challenges for pervasive interaction:

1. Can we devise distributed models for multi-modal fusion and interaction with information on heterogeneous devices?
2. Can we devise models for distributed interaction that migrates over available devices as the user changes location and task?
3. Can we manage migration of interaction over devices in a manner that provides seamless immersive interaction with information, services and media?
4. Can we provide models of distributed interaction that conserve the interaction context as services migrate?

Research Actions for Interaction with Pervasive Smart Objects for the period 2017 - 2020 include

3.4.1. Situated interaction with pervasive displays

The emergence of low-cost interactive displays will enable a confluence of virtual and physical environments. Our goal in this area is to go beyond simple graphical user interfaces in such environments to provide immersive multi-sensorial interaction and communication. A primary concern will be interaction technologies that blend visual with haptic/tactile feedback and 3D interaction and computer vision. We will investigate the use of visual-tactile feedback as well as vibratory signals to augment multi-sensorial interaction and communication. The focus will be on the phenomena of immersive interaction in real worlds that can be made possible by the blending of physical and virtual in ordinary environments.

3.4.2. Wearable and tangible interaction with smart textiles and wearable projectors

Opportunities in this area result from the emergence of new forms of interactive media using smart objects. We will explore the use of smart objects as tangible interfaces that make it possible to experience and interact with information and services by grasping and manipulating objects. We will explore the use of sensors and actuators in clothing and wearable devices such as gloves, hats and wrist bands both as a means of unobtrusively sensing human intentions and emotional states and as a means of stimulating human senses through vibration and sound. We will explore the new forms of interaction and immersion made possible by deploying interactive displays over large areas of an environment.

3.4.3. Pervasive interaction with ecologies of smart objects in the home

In this research area, we will explore and evaluate interaction with ecologies of smart objects in home environments. We will explore development of a range of smart objects that provide information services, such as devices for Episodic Memory for work surfaces and storage areas, devices to provide energy efficient control of environmental conditions, and interactive media that collect and display information. We propose to develop a new class of socially aware managers that coordinate smart objects and manage logistics in functional areas such as the kitchen, living rooms, closets, bedrooms, bathroom or office.

3.4.4. Bibliography

[Van Krevelen 10] D. W. F. Van Krevelen and R. Poelman, A survey of augmented reality technologies, applications and limitations. International Journal of Virtual Reality, 9(2), 1, 2010

POTIOC Project-Team

3. Research Program

3.1. Introduction

The project of team potioc is oriented along three axes:

- Understanding humans interacting with the digital world
- Creating interactive systems
- Exploring new applications and usages

These axes are depicted in Figure 2 .

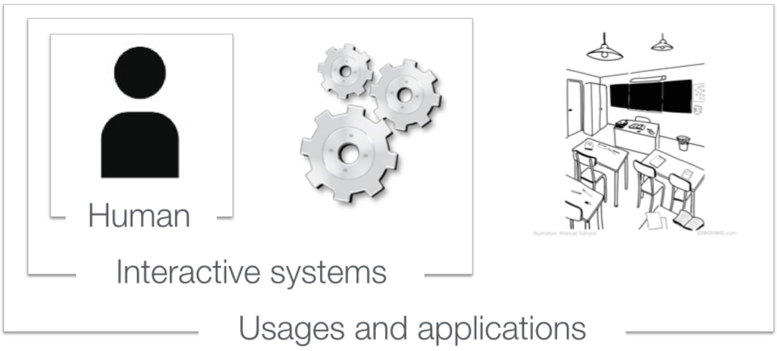

Figure 2. The three axes of the potioc team objectives.

Objective 1 is centered on the human sensori-motor and cognitive abilities, as well as user strategies and preferences, for completing interaction tasks. Our target contribution for this objective are a better understanding of humans interacting with interactive systems. The impact of this objective is mainly at a fundamental level.

In objective 2, our goal is to create interactive systems. This may include hardware parts where new input and output modalities are explored. This also includes software parts, that are strongly linked to the underlying hardware components. Our target contribution in objective 2 is to develop (hardware/software) interaction techniques allowing humans to perform interaction tasks.

Finally, in objective 3, we consider interaction at a higher level, taking into account factors that are linked to specific application domains and usages. Our target contribution in this area is the exploration and the emergence of new applications and usages that take benefit from the results of the project. With this objective, we target mainly a societal impact.

Of course, strong links exist between the three objectives of the project. For example, the results obtained in objective 1 guide the development of objective 2. Conversely, new systems developed in objective 2 may feed research questions of objective 1. There are similar links with objective 3.

3.2. Objective 1: Understanding humans interacting with the digital world

Our first objective is centered on the human side. Our finality is not to enhance the general knowledge about the human being as a research team in psychology would do. Instead, we focus on human skills and behaviors during interaction processes. To this end, we conduct experiments that allow us to better understand what users like, where and why they have difficulties. Thanks to these investigations, we are able to design interaction techniques and systems (described in Objective 2) that are well suited to the targeted users. We believe that this fundamental piece of work is the first step that is required for the design of usable popular interactions. We are particularly interested in 3D interaction tasks for which we design dedicated experiments. We also explore a new approach based on physiological and brain (ElectroEncephaloGraphy - EEG) signals for the evaluation of these interactions.

3.2.1. Interacting with physical and virtual environments

Interacting with digital content displayed on 2D screens has been extensively studied in HCI. On the other hand, less conventional contexts have been studied less. This is the case of 3D environments, immersive virtual environments, augmented reality, and tangible objects. With the final goal of making interaction in such contexts user-friendly, we conduct experiments to better understand user strategies and performance. This allows us to propose guidelines to help designers creating of tools that are accessible to non-expert users.

3.2.2. Evaluating (3D) interaction with physiological signals

Recently, physiological computing has been shown to be a promising complement to Human-Computer Interfaces (HCI) in general, and to 3D User Interfaces (3DUI) in particular, in several directions. Within this research area, we are interested in using various physiological signals, and notably EEG signals, as a new tool to assess objectively the ergonomic quality of a given (3D) UI, to identify where and when are the pros and cons of this interface, based on the user's mental state during interaction. For instance, estimating the user's mental workload during interaction can give insights about where and when the interface is cognitively difficult to use. This could be useful for 2D HCI in general, and even more for 3DUI. Indeed, in a 3DUI, the user perception of the 3D scene – part of which could potentially be measured in EEG - is essential. Moreover, the usual need for a mapping between the user inputs and the corresponding actions on 3D objects make 3DUI and interaction techniques more difficult to assess and to design.

3.2.3. Interacting with Brain-Computer Interfaces

Although very promising for numerous applications, BCIs mostly remain prototypes not used outside laboratories, due to their low reliability. Poor BCI performances are partly due to imperfect EEG signal processing algorithms but also to the user who may not be able to produce reliable EEG patterns. Indeed, BCI use is a skill, requiring the user to be properly trained to achieve BCI control. If he/she cannot perform the desired mental commands, no signal processing algorithm can identify them. Therefore, rather than improving EEG signal processing alone, an interesting research direction is to also guide users to learn BCI control mastery. We aim at addressing this objective. We are notably exploring theoretical models and guidelines from educational sciences to improve BCI training protocols. We also study which users' profiles (personality and cognitive profile) fail or succeed at learning BCI control. Finally, we explore new feedback types and new EEG visualization techniques in order to help users gain BCI control skills more efficiently. These new feedback and visualizations notably aim at providing BCI users with more information about their EEG patterns, in order to identify more easily relevant BCI control strategies, as well as motivating and engaging them in the learning task.

3.2.4. Interaction for people with special needs

Interaction capabilities and needs largely depend on the target user group. In the Potioc project-team, we work with people having special needs. As an example, we work with children in the context of education, which requires us to design interfaces that are usable, engaging and support learning for this target group. Furthermore, we work with people with cognitive or perceptive disabilities, which requires us to consider accessibility, while at the same time designing interfaces that are learnable and enjoyable to use. In order to meet the needs of the different target groups, we apply participative and user-centred design methods.

3.3. Objective 2: Creating interactive systems

Our objective here is to create interactive systems and design interaction techniques dedicated to the completion of interaction tasks. We divide our work into three main categories:

- Interaction techniques based on existing Input/Output (IO) devices.
- New IO and related techniques.
- BCI and physiological computing.

3.3.1. Interaction techniques based on existing Input/Output (IO) devices

When using desktop IOs (i.e., based on mice/keyboards/monitors), a big challenge is to design interaction techniques that allow users to complete 3D interaction tasks. Indeed, the desktop IO space that is mainly dedicated to the completion of 2D interaction task is not well suited to 3D content and, consequently, 3D user interfaces need to be designed with a great care. In the past few years, we have been particularly interested in the problem of interaction when the 3D content is displayed on a touchscreen. Indeed, standard (2D) HCI has evolved from mouse to touch input, and numerous research projects have been conducted. On the contrary, in 3D, very little work has been proposed. We are contributing to moving desktop 3D UIs from the mouse to the touch paradigm; what we used to do with mice in front of a screen does not work well on touch devices anymore. In the future, we will continue designing new interaction techniques that are based on standard IOs (eg. pointing devices and webcams) and that target the main objectives of Potioc which are to enhance the interaction bandwidth for non expert users.

3.3.2. New IO and related techniques

Beyond standard IOs, we are interested in exploring new IO modalities that may make interaction easier, more engaging and motivating. In Potioc, we design new interactive systems that exploit unconventional IO modalities such as stereoscopy, 3D spatial input, augmented reality and so on. In particular, tangible interaction and spatial augmented reality are major subjects of interest for us. Indeed, we believe that manipulating directly physical objects for interacting with the digital world has a great potential, in particular when the general public is targeted. With such approaches, the computer disappears, and the user interacts with the digital content as he or she would do with physical content, which reduces the distance to the manipulated content. As an example, we recently designed Teegi, a new system based on a unique combination of spatial augmented reality, tangible interaction and real-time neurotechnologies. With Teegi, a user can visualize and analyze his or her own brain activity in real-time, on a tangible character that can be easily manipulated, and with which it is possible to interact. Such unconventionnal user interfaces that are based on rich sensing modalities hold great promises in the field of popular interaction.

We are also interested in designing systems that combine different sensory modalities, such as vision, touch and audition. Concrete examples include the design of tangible user interfaces or interfaces for visually impaired people. It has been shown that multimodality can provide rich interaction that can efficiently support learning, and it is also important in the context of accessibility.

3.3.3. BCI and physiological computing

Although Brain-Computer Interfaces (BCI) have demonstrated their tremendous potential in numerous applications, they are still mostly prototypes, not used outside laboratories. This is mainly due to the following limitations:

- Performances: the poor classification accuracies of BCIs make them inconvenient to use or simply useless compared to available alternatives
- Stability and robustness: the sensibility of ElectroEncephaloGraphic (EEG) signals to noise and their inherent non-stationarity make the already poor initial performances difficult to maintain over time
- Calibration time: the need to tune current BCIs to each user's EEG signals makes their calibration times too long.

As part of our research on EEG-based BCIs, we notably aim at addressing these limitations by designing robust EEG signal processing tools with minimal calibration times, in order to design practical BCI systems, usable and useful outside laboratories. To do so we explore the design of alternative features and robust spatial filtering algorithms to make BCIs more robust to noise and non-stationarities, as well as more accurate. We also explore artificial EEG data generation and user-to-user data transfer to reduce calibration times.

3.4. Objective 3: Exploring new applications and usages

Objective 3 is centered on the applications and usages. Beyond the human sensori-motor and cognitive skills (Objective 1), and the hardware and software components (Objective 2), Objectives 3 takes into account broader criteria for the emergence of new usages and applications in various areas, and in particular in the scope of education, art, popularization of science and entertainment. Our goal here is not to develop full-fledged end-user applications. Instead, our contribution is to stimulate the evolution of current applications with new engaging interactive systems.

3.4.1. Education

Education is at the core of the motivations of the Potioc group. Indeed, we are convinced that the approaches we investigate—which target motivation, curiosity, pleasure of use and high level of interactivity—may serve education purposes. To this end, we collaborate with experts in Educational Sciences and teachers for exploring new interactive systems that enhance learning processes. We are currently investigating the fields of astronomy, optics, and neurosciences. We are also working with special education centres for the blind on accessible augmented reality prototypes. In the future, we will continue exploring new interactive approaches dedicated to education, in various fields.

3.4.2. Popularization of science

Popularization of Science is also a key domain for Potioc. Focusing on this subject allows us to get inspiration for the development of new interactive approaches. In particular, we have built a strong partnership with Cap Sciences, which is a center dedicated to the popularization of science in Bordeaux that is visited by thousands of visitors every month. This was initiated with the ANR national project InSTInCT, whose goal was to study the benefits of 3D touch-based interaction in public exhibitions. This project has led to the creation of a Living Lab where several systems developed by Potioc have been tested and will be tested by the visitors. This provides us with very interesting observations that go beyond the feedback we can obtain in our controlled lab-experiments.

3.4.3. Art

Art, which is strongly linked with emotions and user experiences, is also a target area for Potioc. We believe that the work conducted in Potioc may be beneficial for creation from the artist point of view, and it may open new interactive experiences from the audience point of view. As an example, we are working with colleagues who are specialists in digital music, and with musicians. We are also working with jugglers and mockup builders with the goal of enhancing interactivity and user experience.

3.4.4. Entertainment

Similarly, entertainment is a domain where our work may have an impact. We notably explored BCI-based gaming and non-medical applications of BCI, as well as mobile Augmented Reality games. Once again, we believe that our approaches that merge the physical and the virtual world may enhance the user experience. Exploring such a domain will raise numerous scientific and technological questions.

RITS Project-Team

3. Research Program

3.1. Vehicle guidance and autonomous navigation

Participants: Zayed Alsayed, Pierre de Beaucorps, Raoul de Charette, Rafael Colmenares Prieto, Aitor Gomez Torres, Fernando Garrido Carpio, David González Bautista, Pierre Merdrignac, Alexis Meyer, Vicente Milanés, Francisco Navas, Fawzi Nashashibi, Carlos Flores, Dinh-Van Nguyen, Danut-Ovidiu Pop, Oyunchimeg Shagdar, Thomas Streubel, Guillaume Trehard, Anne Verroust-Blondet, Itheri Yahiaoui.

There are three basic ways to improve the safety of road vehicles and these ways are all of interest to the project-team. The first way is to assist the driver by giving him better information and warning. The second way is to take over the control of the vehicle in case of mistakes such as inattention or wrong command. The third way is to completely remove the driver from the control loop.

All three approaches rely on information processing. Only the last two involve the control of the vehicle with actions on the actuators, which are the engine power, the brakes and the steering. The research proposed by the project-team is focused on the following elements:

- perception of the environment,
- planning of the actions,
- real-time control.

3.1.1. Perception of the road environment

Participants: Zayed Alsayed, Raoul de Charette, Rafael Colmenares Prieto, Aitor Gomez Torres, Pierre Merdrignac, Alexis Meyer, Fawzi Nashashibi, Dinh-Van Nguyen, Danut-Ovidiu Pop, Guillaume Trehard, Anne Verroust-Blondet, Itheri Yahiaoui.

Either for driver assistance or for fully automated guided vehicle purposes, the first step of any robotic system is to perceive the environment in order to assess the situation around itself. Proprioceptive sensors (accelerometer, gyrometer,...) provide information about the vehicle by itself such as its velocity or lateral acceleration. On the other hand, exteroceptive sensors, such as video camera, laser or GPS devices, provide information about the environment surrounding the vehicle or its localization. Obviously, fusion of data with various other sensors is also a focus of the research.
The following topics are already validated or under development in our team:

- relative ego-localization with respect to the infrastructure, i.e. lateral positioning on the road can be obtained by mean of vision (lane markings) and the fusion with other devices (e.g. GPS);
- global ego-localization by considering GPS measurement and proprioceptive information, even in case of GPS outage;
- road detection by using lane marking detection and navigable free space;
- detection and localization of the surrounding obstacles (vehicles, pedestrians, animals, objects on roads, etc.) and determination of their behavior can be obtained by the fusion of vision, laser or radar based data processing;
- simultaneous localization and mapping as well as mobile object tracking using laser-based and stereovision-based (SLAMMOT) algorithms.

Scene understanding is a large perception problem. In this research axis we have decided to use only computer vision as cameras have evolved very quickly and can now provide much more precise sensing of the scene, and even depth information. Two types of hardware setups were used, namely: monocular vision or stereo vision to retrieve depth information which allow extracting geometry information.

We have initiated several works:

- estimation of the ego motion using monocular scene flow. Although in the state of the art most of the algorithms use a stereo setup, researches were conducted to estimate the ego-motion using a novel approach with a strong assumption.
- bad weather conditions evaluations. Most often all computer vision algorithms work under a transparent atmosphere assumption which assumption is incorrect in the case of bad weather (rain, snow, hail, fog, etc.). In these situations the light ray are disrupted by the particles in suspension, producing light attenuation, reflection, refraction that alter the image processing.
- deep learning for object recognition. New works are being initiated in our team to develop deep learning recognition in the context of heterogeneous data.

3.1.2. Cooperative Multi-sensor data fusion

Participants: Pierre Merdrignac, Fawzi Nashashibi, Oyunchimeg Shagdar.

Since data are noisy, inaccurate and can also be unreliable or unsynchronized, the use of data fusion techniques is required in order to provide the most accurate situation assessment as possible to perform the perception task. RITS team worked a lot on this problem in the past, but is now focusing on collaborative perception approach. Indeed, the use of vehicle-to-vehicle or vehicle-to-infrastructure communications allows an improved on-board reasoning since the decision is made based on an extended perception.

As a direct consequence of the electronics broadly used for vehicular applications, communication technologies are now being adopted as well. In order to limit injuries and to share safety information, research in driving assistance system is now orientating toward the cooperative domain. Advanced Driver Assistance System (ADAS) and Cybercars applications are moving towards vehicle-infrastructure cooperation. In such scenario, information from vehicle based sensors, roadside based sensors and a priori knowledge is generally combined thanks to wireless communications to build a probabilistic spatio-temporal model of the environment. Depending on the accuracy of such model, very useful applications from driver warning to fully autonomous driving can be performed.

The Collaborative Perception Framework (CPF) is a combined hardware/software approach that permits to see remote information as its own information. Using this approach, a communicant entity can see another remote entity software objects as if it was local, and a sensor object, can see sensor data of others entities as its own sensor data. Last year we developed the basic hardware modules that ensure the well functioning of the embedded architecture including perception sensors, communication devices and processing tools.

Finally, since vehicle localization (ground vehicles) is an important task for intelligent vehicle systems, vehicle cooperation may bring benefits for this task. A new cooperative multi-vehicle localization method using split covariance intersection filter was developed during the year 2012, as well as a cooperative GPS data sharing method.

In the first method, each vehicle estimates its own position using a SLAM (Simultaneous Localization And Mapping) approach. In parallel, it estimates a decomposed group state, which is shared with neighboring vehicles; the estimate of the decomposed group state is updated with both the sensor data of the ego-vehicle and the estimates sent from other vehicles; the covariance intersection filter which yields consistent estimates even facing unknown degree of inter-estimate correlation has been used for data fusion.

In the second GPS data sharing method, a new collaborative localization method is proposed. On the assumption that the distance between two communicative vehicles can be calculated with a good precision, cooperative vehicle are considered as additional satellites into the user position calculation by using iterative methods. In order to limit divergence, some filtering process is proposed: Interacting Multiple Model (IMM) is used to guarantee a greater robustness in the user position estimation.

Accidents between vehicles and pedestrians (including cyclists) often result in fatality or at least serious injury for pedestrians, showing the need of technology to protect vulnerable road users. Vehicles are now equipped with many sensors in order to model their environment, to localize themselves, detect and classify obstacles, etc. They are also equipped with communication devices in order to share the information with other road users and the environment. The goal of this work is to develop a cooperative perception and communication system, which merges information coming from the communications device and obstacle detection module to improve the pedestrian detection, tracking, and hazard alarming.

Pedestrian detection is performed by using a perception architecture made of two sensors: a laser scanner and a CCD camera. The laser scanner provides a first hypothesis on the presence of a pedestrian-like obstacle while the camera performs the real classification of the obstacle in order to identify the pedestrian(s). This is a learning-based technique exploiting adaptive boosting (AdaBoost). Several classifiers were tested and learned in order to determine the best compromise between the nature and the number of classifiers and the accuracy of the classification.

3.1.3. Planning and executing vehicle actions

Participants: Fernando Garrido Carpio, David González Bautista, Vicente Milanés, Fawzi Nashashibi, Francisco Navas, Carlos Flores.

From the understanding of the environment, thanks to augmented perception, we have either to warn the driver to help him in the control of his vehicle, or to take control in case of a driverless vehicle. In simple situations, the planning might also be quite simple, but in the most complex situations we want to explore, the planning must involve complex algorithms dealing with the trajectories of the vehicle and its surroundings (which might involve other vehicles and/or fixed or moving obstacles). In the case of fully automated vehicles, the perception will involve some map building of the environment and obstacles, and the planning will involve partial planning with periodical recomputation to reach the long term goal. In this case, with vehicle to vehicle communications, what we want to explore is the possibility to establish a negotiation protocol in order to coordinate nearby vehicles (what humans usually do by using driving rules, common sense and/or non verbal communication). Until now, we have been focusing on the generation of geometric trajectories as a result of a maneuver selection process using grid-based rating technique or fuzzy technique. For high speed vehicles, Partial Motion Planning techniques we tested, revealed their limitations because of the computational cost. The use of quintic polynomials we designed, allowed us to elaborate trajectories with different dynamics adapted to the driver profile. These trajectories have been implemented and validated in the JointSystem demonstrator of the German Aerospace Center (DLR) used in the European project HAVEit, as well as in RITS's electrical vehicle prototype used in the French project ABV. HAVEit was also the opportunity for RITS to take in charge the implementation of the Co-Pilot system which processes perception data in order to elaborate the high level command for the actuators. These trajectories were also validated on RITS's cybercars. However, for the low speed cybercars that have pre-defined itineraries and basic maneuvers, it was necessary to develop a more adapted planning and control system. Therefore, we have developed a nonlinear adaptive control for automated overtaking maneuver using quadratic polynomials and Lyapunov function candidate and taking into account the vehicles kinematics. For the global mobility systems we are developing, the control of the vehicles includes also advanced platooning, automated parking, automated docking, etc. For each functionality a dedicated control algorithm was designed (see publication of previous years). Today, RITS is also investigating the opportunity of fuzzy-based control for specific maneuvers. First results have been recently obtained for reference trajectories following in roundabouts and normal straight roads.

3.2. V2V and V2I Communications for ITS

Participants: Thierry Ernst, Oyunchimeg Shagdar, Gérard Le Lann, Pierre Merdrignac, Mohammad Abualhoul, Fawzi Nashashibi.

Wireless communications are expected to play an important role for road safety, road efficiency, and comfort of road users. Road safety applications often require highly responsive and reliable information exchange between neighboring vehicles in any road density condition. Because the performance of the existing radio communications technology largely degrades with the increase of the node density, the challenge of designing wireless communications for safety applications is enabling reliable communications in highly dense scenarios. Targeting this issue, RITS has been working on medium access control design and visible light communications, especially for highly dense scenarios. The works have been carried out considering the vehicle behavior such as vehicle merging and vehicle platooning.

Unlike many of the road safety applications, the applications regarding road efficiency and comfort of road users, on the other hand, often require connectivity to the Internet. Based on our expertise in both Internet-based communications in the mobility context and in ITS, we are now investigating the use of IPv6 (Internet Protocol version 6 which is going to replace the current version, IPv4, in a few years from now) for vehicular communications, in a combined architecture allowing both V2V and V2I.

The wireless channel and the topology dynamics need to be studied when understanding the dynamics and designing efficient communications mechanisms. Targeting this issue, we have been working on channel modeling for both radio and visible light communications, and design of communications mechanisms especially for security, service discovery, multicast and geocast message delivery, and access point selection.

Below follows a more detailed description of the related research issues.

3.2.1. Geographic multicast addressing and routing

Participants: Oyunchimeg Shagdar, Thierry Ernst.

Many ITS applications such as fleet management require multicast data delivery. Existing work on this subject tackles mainly the problems of IP multicasting inside the Internet or geocasting in the VANETs. To enable Internet-based multicast services for VANETs, we introduced a framework that:
i) defines a distributed and efficient geographic multicast auto-addressing mechanism to ensure vehicular multicast group reachability through the infrastructure network,
ii) introduces a simplified approach that locally manages the group membership and distributes the packets among them to allow simple and efficient data delivery.

3.2.2. Platooning control using visible light communications

Participants: Mohammad Abualhoul, Oyunchimeg Shagdar, Fawzi Nashashibi.

The main purpose of our research is to propose and test new successful supportive communication technology, which can provide stable and reliable communication between vehicles, especially for the platooning scenario. Although VLC technology has a short history in comparison with other communication technologies, the infrastructure availability and the presence of the congestion in wireless communication channels lead to propose VLC technology as a reliable and supportive technology which can takeoff some loads of the wireless radio communication. The first objective of this work is to develop an analytical model of VLC to understand its characteristics and limitations. The second objective is to design vehicle platooning control using VLC. In platooning control, a cooperation between control and communication is strongly required in order to guarantee the platoon's stability (e.g. string stability problem). For this purpose we work on VLC model platooning scenario, to permit for each vehicle the trajectory tracking of the vehicle ahead, altogether with a prescribed inter-vehicle distance and considering all the VLC channel model limitations. The integrated channel model of the main Simulink platooning model will be responsible for deciding the availability of the Line-of-Sight for different trajectory's curvatures, which means the capability of using light communication between each couple of vehicles in the platooning queue. At the same time the model will compute all the required parameters acquired from each vehicle controller.

3.2.3. V2X radio communications for road safety applications

Participants: Mohammad Abualhoul, Pierre Merdrignac, Oyunchimeg Shagdar, Fawzi Nashashibi.

While 5.9 GHz radio frequency band is dedicated to ITS applications, the channel and network behaviors in mobile scenarios are not very well known. In this work we theoretically and experimentally study the radio channel characteristics in vehicular networks, especially the radio quality and bandwidth availability. Based on our study, we develop mechanisms for efficient and reliable V2X communications, channel allocation, congestion control, and access point selection, which are especially dedicated to road safety and autonomous driving applications.

3.2.4. Safety-critical communications in intelligent vehicular networks

Participant: Gérard Le Lann.

Intelligent vehicular networks (IVNs) are constituents of ITS. IVNs range from platoons with a lead vehicle piloted by a human driver to fully ad-hoc vehicular networks, a.k.a. VANETs, comprising autonomous/automated vehicles. Safety issues in IVNs appear to be the least studied in the ITS domain. The focus of our work is on safety-critical (SC) scenarios, where accidents and fatalities inevitably occur when such scenarios are not handled correctly. In addition to on-board robotics, inter-vehicular radio communications have been considered for achieving safety properties. Since both technologies have known intrinsic limitations (in addition to possibly experiencing temporary or permanent failures), using them redundantly is mandatory for meeting safety regulations. Redundancy is a fundamental design principle in every SC cyber-physical domain, such as, e.g., air transportation. (Optics-based inter-vehicular communications may also be part of such redundant constructs.) The focus of our on-going work is on safety-critical (SC) communications. We consider IVNs on main roads and highways, which are settings where velocities can be very high, thus exacerbating safety problems acceptable delays in the cyber space, and response times in the physical space, shall be very small. Human lives being at stake, such delays and response times must have strict (non-stochastic) upper bounds under worst-case conditions (vehicular density, concurrency and failures). Consequently, we are led to look for deterministic solutions.

Rationale

In the current ITS literature, the term *safety* is used without being given a precise definition. That must be corrected. In our case, a fundamental open question is: what is the exact meaning of *SC communications*? We have devised a definition, referred to as space-time bounds acceptability (STBA) requirements. For any given problem related to SC communications, those STBA requirements serve as yardsticks for distinguishing acceptable solutions from unacceptable ones with respect to safety. In conformance with the above, STBA requirements rest on the following worst-case upper bounds: λ for channel access delays, and Δ for distributed inter-vehicular coordination (message dissemination, distributed agreement).

Via discussions with foreign colleagues, notably those active in the IEEE 802 Committee, we have comforted our early diagnosis regarding existing standards for V2V/V2I/V2X communications, such as IEEE 802.11p and ETSI ITS-G5: they are totally inappropriate regarding SC communications. A major flaw is the choice of CSMA/CA as the MAC-level protocol. Obviously, there cannot be such bounds as λ and Δ with CSMA/CA. Another flaw is the choice of medium-range omnidirectional communications, radio range in the order of 250 m, and interference range in the order of 400 m. Stochastic delays achievable with existing standards are just unacceptable in moderate/worst-case contention conditions. Consider the following setting, not uncommon in many countries: a highway, 3 lanes each direction, dense traffic, i.e. 1 vehicle per 12.5 m. A simple calculation leads to the following result: any vehicle may experience (destructive) interferences from up to 384 vehicles. Even if one assumes some reasonable communications activity ratio, say 25%, one finds that up to 96 vehicles may be contending for channel access. Under such conditions, MAC-level delays and string-wide dissemination/agreement delays achieved by current standards fail to meet the STBA requirements by huge margins.

Reliance on V2I communications via terrestrial infrastructures and nodes, such as road-side units or WiFi hotspots, rather than direct V2V communications, can only lead to poorer results. First, reachability is not guaranteed: hazardous conditions may develop anywhere anytime, far away from a terrestrial node. Second, mixing SC communications and ordinary communications within terrestrial nodes is a violation of the very fundamental segregation principle: SC communications and processing shall be isolated from ordinary communications and processing. Third, security: it is very easy to jam or to spy on a terrestrial node; moreover, terrestrial nodes may be used for launching all sorts of attacks, man-in-the-middle attacks for example. Fourth, delays can only get worse than with direct V2V communications, since transiting via a node inevitably introduces additional latencies. Fifth, the delivery of every SC message must be acknowledged, which exacerbates the latency problems. Sixth, availability: what happens when a terrestrial node fails?

Trying to tweak existing standards for achieving SC communications is vain. That is also unjustified. Clearly, medium-range omnidirectional communications are unjustified for the handling of SC scenarios. By definition, accidents can only involve vehicles that are very close to each other. Therefore, short-range directional communications suffice. The obvious conclusion is that novel protocols and inter-vehicular coordination algorithms based on short-range direct V2V communications are needed. It is mandatory to check whether these novel solutions meet the STBA requirements. Future standards specifically aimed at SC communications in IVNs may emerge from such solutions.

Naming and privacy

Additionally, we are exploring the (re)naming problem as it arises in IVNs. Source and destination names appear in messages exchanged among vehicles. Most often, names are IP addresses or MAC addresses (plate numbers shall not be used for privacy reasons). A vehicle which intends to communicate with some vehicle, denoted V here, must know which name *name(V)* to use in order to reach/designate V. Existing solutions are based on multicasting/broadcasting existential messages, whereby every vehicle publicizes its existence (name and geolocation), either upon request (replying to a Geocast) or spontaneously (periodic beaconing). These solutions have severe drawbacks. First, they contribute to overloading communication channels (leading to unacceptably high worst-case delays). Second, they amount to breaching privacy voluntarily. Why should vehicles reveal their existence and their time dependent geolocations, making tracing and spying much easier? Novel solutions are needed. They shall be such that:

- At any time, a vehicle can assign itself a name that is unique within a geographical zone centered on that vehicle (no third-party involved),
- No linkage may exist between a name and those identifiers (plate numbers, IP/MAC addresses, etc.) proper to a vehicle,
- Different (unique) names can be computed at different times by a vehicle (names can be short-lived or long-lived),
- *name(V)* at UTC time t is revealed only to those vehicles sufficiently close to V at time t, notably those which may collide with V.

We have solved the (re)naming problem in string/cohort formations [48]. Ranks (unique integers in any given string/cohort) are privacy-preserving names, easily computed by every member of a string, in the presence of string membership changes (new vehicles join in, members leave). That problem is open when considering arbitrary clusters of vehicles/strings encompassing multiple lanes.

3.3. Probabilistic modeling for large transportation systems

Participants: Guy Fayolle, Jean-Marc Lasgouttes.

This activity concerns the modeling of random systems related to ITS, through the identification and development of solutions based on probabilistic methods and more specifically through the exploration of links between large random systems and statistical physics. Traffic modeling is a very fertile area of application for this approach, both for macroscopic (fleet management [46], traffic prediction) and for microscopic (movement of each vehicle, formation of traffic jams) analysis. When the size or volume of structures grows (leading to the so-called "thermodynamic limit"), we study the quantitative and qualitative (performance, speed, stability, phase transitions, complexity, etc.) features of the system.

In the recent years, several directions have been explored.

3.3.1. Traffic reconstruction

Large random systems are a natural part of macroscopic studies of traffic, where several models from statistical physics can be fruitfully employed. One example is fleet management, where one main issue is to find optimal ways of reallocating unused vehicles: it has been shown that Coulombian potentials might be an efficient tool to drive the flow of vehicles. Another case deals with the prediction of traffic conditions, when the data comes from probe vehicles instead of static sensors.

While the widely-used macroscopic traffic flow models are well adapted to highway traffic, where the distance between junction is long (see for example the work done by the NeCS team in Grenoble), our focus is on a more urban situation, where the graphs are much denser. The approach we are advocating here is model-less, and based on statistical inference rather than fundamental diagrams of road segments. Using the Ising model or even a Gaussian Random Markov Field, together with the very popular Belief Propagation (BP) algorithm, we have been able to show how real-time data can be used for traffic prediction and reconstruction (in the space-time domain).

This new use of BP algorithm raises some theoretical questions about the ways the make the belief propagation algorithm more efficient:

- find the best way to inject real-valued data in an Ising model with binary variables [50];
- build macroscopic variables that measure the overall state of the underlying graph, in order to improve the local propagation of information [47];
- make the underlying model as sparse as possible, in order to improve BP convergence and quality [49].

3.3.2. Exclusion processes for road traffic modeling

The focus here is on road traffic modeled as a granular flow, in order to analyze the features that can be explained by its random nature. This approach is complementary to macroscopic models of traffic flow (as done for example in the Opale team at Inria), which rely mainly on ODEs and PDEs to describe the traffic as a fluid.

One particular feature of road traffic that is of interest to us is the spontaneous formation of traffic jams. It is known that systems as simple as the Nagel-Schreckenberg model are able to describe traffic jams as an emergent phenomenon due to interaction between vehicles. However, even this simple model cannot be explicitly analyzed and therefore one has to resort to simulation.

One of the simplest solvable (but non trivial) probabilistic models for road traffic is the exclusion process. It lends itself to a number of extensions allowing to tackle some particular features of traffic flows: variable speed of particles, synchronized move of consecutive particles (platooning), use of geometries more complex than plain 1D (cross roads or even fully connected networks), formation and stability of vehicle clusters (vehicles that are close enough to establish an ad-hoc communication system), two-lane roads with overtaking.

The aspect that we have particularly studied is the possibility to let the speed of vehicle evolve with time. To this end, we consider models equivalent to a series of queues where the pair (service rate, number of customers) forms a random walk in the quarter plane $\mathbb{Z}_+^2$.

Having in mind a global project concerning the analysis of complex systems, we also focus on the interplay between discrete and continuous description: in some cases, this recurrent question can be addressed quite rigorously via probabilistic methods.

We have considered in [43] some classes of models dealing with the dynamics of discrete curves subjected to stochastic deformations. It turns out that the problems of interest can be set in terms of interacting exclusion processes, the ultimate goal being to derive hydrodynamic limits after proper scaling. A seemingly new method is proposed, which relies on the analysis of specific partial differential operators, involving variational calculus and functional integration. Starting from a detailed analysis of the Asymmetric Simple Exclusion Process (ASEP) system on the torus $\mathbb{Z}/n\mathbb{Z}$, the arguments a priori work in higher dimensions (ABC, multi-type exclusion processes, etc), leading to systems of coupled partial differential equations of Burgers' type.

3.3.3. Random walks in the quarter plane $\mathbb{Z}_+^2$

This field remains one of the important *"violon d'Ingres"* in our research activities in stochastic processes, both from theoretical and applied points of view. In particular, it is a building block for models of many communication and transportation systems.

One essential question concerns the computation of stationary measures (when they exist). As for the answer, it has been given by original methods formerly developed in the team (see books and related bibliography). For instance, in the case of small steps (jumps of size one in the interior of $\mathbb{Z}_+^2$), the invariant measure $\{\pi_{i,j}, i,j \geq 0\}$ does satisfy the fundamental functional equation (see [45]):

$$Q(x,y)\pi(x,y) = q(x,y)\pi(x) + \widetilde{q}(x,y)\widetilde{\pi}(y) + \pi_0(x,y). \tag{96}$$

where the unknown generating functions $\pi(x,y), \pi(x), \widetilde{\pi}(y), \pi_0(x,y)$ are sought to be analytic in the region $\{(x,y) \in \mathbb{C}^2 : |x| < 1, |y| < 1\}$, and continuous on their respective boundaries.

The given function $Q(x,y) = \sum_{i,j} p_{i,j} x^i y^j - 1$, where the sum runs over the possible jumps of the walk inside $\mathbb{Z}_+^2$, is often referred to as the *kernel*. Then it has been shown that equation (1) can be solved by reduction to a boundary-value problem of Riemann-Hilbert type. This method has been the source of numerous and fruitful developments. Some recent and ongoing works have been dealing with the following matters.

- *Group of the random walk*. In several studies, it has been noticed that the so-called *group of the walk* governs the behavior of a number of quantities, in particular through its *order*, which is always even. In the case of small jumps, the algebraic curve R defined by $\{Q(x,y) = 0\}$ is either of *genus* 0 (the sphere) or 1 (the torus). In [Fayolle-2011a], when the drift of the random walk is equal to 0 (and then so is the genus), an effective criterion gives the *order* of the group. More generally, it is also proved that whenever the genus is 0, this order is infinite, except precisely for the zero drift case, where finiteness is quite possible. When the *genus* is 1, the situation is more difficult. Recently [44], a criterion has been found in terms of a determinant of order 3 or 4, depending on the arity of the group.
- *Nature of the counting generating functions*. Enumeration of planar lattice walks is a classical topic in combinatorics. For a given set of allowed jumps (or steps), it is a matter of counting the number of paths starting from some point and ending at some arbitrary point in a given time, and possibly restricted to some regions of the plane. A first basic and natural question arises: how many such paths exist? A second question concerns the nature of the associated counting generating functions (CGF): are they rational, algebraic, holonomic (or D-finite, i.e. solution of a linear differential equation with polynomial coefficients)?

  Let $f(i,j,k)$ denote the number of paths in $\mathbb{Z}_+^2$ starting from $(0,0)$ and ending at (i,j) at time k. Then the corresponding CGF

  $$F(x,y,z) = \sum_{i,j,k \geq 0} f(i,j,k) x^i y^j z^k \tag{97}$$

  satisfies the functional equation

  $$K(x,y)F(x,y,z) = c(x)F(x,0,z) + \widetilde{c}(y)F(0,y,z) + c_0(x,y), \tag{98}$$

where z is considered as a time-parameter. Clearly, equations (2) and (1) are of the same nature, and answers to the above questions have been given in [Fayolle-2010].

- *Some exact asymptotics in the counting of walks in* $\mathbb{Z}_+^2$. A new and uniform approach has been proposed about the following problem: *What is the asymptotic behavior, as their length goes to infinity, of the number of walks ending at some given point or domain (for instance one axis)?* The method in [Fayolle-2012] works for *both* finite or infinite groups, and for walks not necessarily restricted to excursions.

3.3.4. Discrete-event simulation for urban mobility

We have developed two simulation tools to study and evaluate the performance of different transportation modes covering an entire urban area.

- one for collective taxis, a public transportation system with a service quality provided will be comparable with that of conventional taxis (system operating with or without reservations, door-to-door services, well adapted itineraries following the current demand, controlling detours and waits, etc.), and with fares set at rates affordable by almost everyone, simply by utilizing previously wasted vehicle capacity;
- the second for a system of self-service cars that can reconfigure themselves into shuttles, therefore creating a multimodal public transportation system; this second simulator is intended to become a generic tool for multimodal transportation.

These two programs use a technique allowing to run simulations in batch mode and analyze the dynamics of the system afterward.

SEMAGRAMME Project-Team

3. Research Program

3.1. Overview

The Sémagramme project relies on deep mathematical foundations. We intend to develop models based on well-established mathematics. We seek two main advantages from this approach. On the one hand, by relying on mature theories, we have at our disposal sets of mathematical tools that we can use to study our models. On the other hand, developing various models on a common mathematical background will make them easier to integrate, and will ease the search for unifying principles.

The main mathematical domains on which we rely are formal language theory, symbolic logic, and type theory.

3.2. Formal language theory

Formal language theory studies the purely syntactic and combinatorial aspects of languages, seen as sets of strings (or possibly trees or graphs). Formal language theory has been especially fruitful for the development of parsing algorithms for context-free languages. We use it, in a similar way, to develop parsing algorithms for formalisms that go beyond context-freeness. Language theory also appears to be very useful in formally studying the expressive power and the complexity of the models we develop.

3.3. Symbolic logic

Symbolic logic (and, more particularly, proof-theory) is concerned with the study of the expressive and deductive power of formal systems. In a rule-based approach to computational linguistics, the use of symbolic logic is ubiquitous. As we previously said, at the level of syntax, several kinds of grammars (generative, categorial...) may be seen as basic deductive systems. At the level of semantics, the meaning of an utterance is captured by computing (intermediate) semantic representations that are expressed as logical forms. Finally, using symbolic logics allows one to formalize notions of inference and entailment that are needed at the level of pragmatics.

3.4. Type theory and typed λ-calculus

Among the various possible logics that may be used, Church's simply typed λ-calculus and simple theory of types (a.k.a. higher-order logic) play a central part. On the one hand, Montague semantics is based on the simply typed λ-calculus, and so is our syntax-semantics interface model. On the other hand, as shown by Gallin [39], the target logic used by Montague for expressing meanings (i.e., his intensional logic) is essentially a variant of higher-order logic featuring three atomic types (the third atomic type standing for the set of possible worlds).

SIROCCO Project-Team

3. Research Program

3.1. Introduction

The research activities on analysis, compression and communication of visual data mostly rely on tools and formalisms from the areas of statistical image modelling, of signal processing, of coding and information theory. However, the objective of better exploiting the Human Visual System (HVS) properties in the above goals also pertains to the areas of perceptual modelling and cognitive science. Some of the proposed research axes are also based on scientific foundations of computer vision (e.g. multi-view modelling and coding). We have limited this section to some tools which are central to the proposed research axes, but the design of complete compression and communication solutions obviously rely on a large number of other results in the areas of motion analysis, transform design, entropy code design, etc which cannot be all described here.

3.2. Parameter Estimation and Inference

Bayesian estimation, Expectation-Maximization, stochastic modelling

Parameter estimation is at the core of the processing tools studied and developed in the team. Applications range from the prediction of missing data or future data, to extracting some information about the data in order to perform efficient compression. More precisely, the data are assumed to be generated by a given stochastic data model, which is partially known. The set of possible models translates the a priori knowledge we have on the data and the best model has to be selected in this set. When the set of models or equivalently the set of probability laws is indexed by a parameter (scalar or vectorial), the model is said parametric and the model selection resorts to estimating the parameter. Estimation algorithms are therefore widely used at the encoder to analyze the data. In order to achieve high compression rates, the parameters are usually not sent and the decoder has to jointly select the model (i.e. estimate the model parameters) and extract the information of interest.

3.3. Data Dimensionality Reduction

Manifolds, locally linear embedding, non-negative matrix factorization, principal component analysis

A fundamental problem in many data processing tasks (compression, classification, indexing) is to find a suitable representation of the data. It often aims at reducing the dimensionality of the input data so that tractable processing methods can then be applied. Well-known methods for data dimensionality reduction include principal component analysis (PCA) and independent component analysis (ICA). The methodologies which will be central to several proposed research problems will instead be based on sparse representations, on locally linear embedding (LLE) and on the “non negative matrix factorization” (NMF) framework.

The objective of *sparse representations* is to find a sparse approximation of a given input data. In theory, given $A \in \mathbb{R}^{m \times n}$, $m < n$, and $\mathbf{b} \in \mathbb{R}^m$ with $m << n$ and A is of full rank, one seeks the solution of $\min\{\|\mathbf{x}\|_0 \ : \ A\mathbf{x} = \mathbf{b}\}$, where $\|\mathbf{x}\|_0$ denotes the L_0 norm of x, i.e. the number of non-zero components in z. There exist many solutions x to $Ax = b$. The problem is to find the sparsest, the one for which x has the fewest non zero components. In practice, one actually seeks an approximate and thus even sparser solution which satisfies $\min\{\|\mathbf{x}\|_0 \ : \ \|A\mathbf{x} - \mathbf{b}\|_p \leq \rho\}$, for some $\rho \geq 0$, characterizing an admissible reconstruction error. The norm p is usually 2, but could be 1 or ∞ as well. Except for the exhaustive combinatorial approach, there is no known method to find the exact solution under general conditions on the dictionary A. Searching for this sparsest representation is hence unfeasible and both problems are computationally intractable. Pursuit algorithms have been introduced as heuristic methods which aim at finding approximate solutions to the above problem with tractable complexity.

Non negative matrix factorization (NMF) is a non-negative approximate data representation [0]. NMF aims at finding an approximate factorization of a non-negative input data matrix V into non-negative matrices W and H, where the columns of W can be seen as *basis vectors* and those of H as coefficients of the linear approximation of the input data. Unlike other linear representations like PCA and ICA, the non-negativity constraint makes the representation purely additive. Classical data representation methods like PCA or Vector Quantization (VQ) can be placed in an NMF framework, the differences arising from different constraints being placed on the W and H matrices. In VQ, each column of H is constrained to be unitary with only one non-zero coefficient which is equal to 1. In PCA, the columns of W are constrained to be orthonormal and the rows of H to be orthogonal to each other. These methods of data-dependent dimensionality reduction will be at the core of our visual data analysis and compression activities.

3.4. Perceptual Modelling

Saliency, visual attention, cognition

The human visual system (HVS) is not able to process all visual information of our visual field at once. To cope with this problem, our visual system must filter out irrelevant information and reduce redundant information. This feature of our visual system is driven by a selective sensing and analysis process. For instance, it is well known that the greatest visual acuity is provided by the fovea (center of the retina). Beyond this area, the acuity drops down with the eccentricity. Another example concerns the light that impinges on our retina. Only the visible light spectrum lying between 380 nm (violet) and 760 nm (red) is processed. To conclude on the selective sensing, it is important to mention that our sensitivity depends on a number of factors such as the spatial frequency, the orientation or the depth. These properties are modeled by a sensitivity function such as the Contrast Sensitivity Function (CSF).

Our capacity of analysis is also related to our visual attention. Visual attention which is closely linked to eye movement (note that this attention is called *overt* while the covert attention does not involve eye movement) allows us to focus our biological resources on a particular area. It can be controlled by both top-down (i.e. goal-directed, intention) and bottom-up (stimulus-driven, data-dependent) sources of information [0]. This detection is also influenced by prior knowledge about the environment of the scene [0]. Implicit assumptions related to prior knowledge or beliefs play an important role in our perception (see the example concerning the assumption that light comes from above-left). Our perception results from the combination of prior beliefs with data we gather from the environment. A Bayesian framework is an elegant solution to model these interactions [0]. We define a vector $\overrightarrow{v}_l$ of local measurements (contrast of color, orientation, etc.) and vector $\overrightarrow{v}_c$ of global and contextual features (global features, prior locations, type of the scene, etc.). The salient locations S for a spatial position $\overrightarrow{x}$ are then given by:

$$S(\overrightarrow{x}) = \frac{1}{p(\overrightarrow{v}_l \,|\, \overrightarrow{v}_c)} \times p(s, \overrightarrow{x} \,|\, \overrightarrow{v}_c) \tag{99}$$

The first term represents the bottom-up salience. It is based on a kind of contrast detection, following the assumption that rare image features are more salient than frequent ones. Most of existing computational models of visual attention rely on this term. However, different approaches exist to extract the local visual features as well as the global ones. The second term is the contextual priors. For instance, given a scene, it indicates which parts of the scene are likely the most salient.

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3.5. Coding theory

OPTA limit (Optimum Performance Theoretically Attainable), Rate allocation, Rate-Distortion optimization, lossy coding, joint source-channel coding multiple description coding, channel modelization, oversampled frame expansions, error correcting codes.

Source coding and channel coding theory [0] is central to our compression and communication activities, in particular to the design of entropy codes and of error correcting codes. Another field in coding theory which has emerged in the context of sensor networks is Distributed Source Coding (DSC). It refers to the compression of correlated signals captured by different sensors which do not communicate between themselves. All the signals captured are compressed independently and transmitted to a central base station which has the capability to decode them jointly. DSC finds its foundation in the seminal Slepian-Wolf [0] (SW) and Wyner-Ziv [0] (WZ) theorems. Let us consider two binary correlated sources X and Y. If the two coders communicate, it is well known from Shannon's theory that the minimum lossless rate for X and Y is given by the joint entropy $H(X,Y)$. Slepian and Wolf have established in 1973 that this lossless compression rate bound can be approached with a vanishing error probability for long sequences, even if the two sources are coded separately, provided that they are decoded jointly and that their correlation is known to both the encoder and the decoder.

In 1976, Wyner and Ziv considered the problem of coding of two correlated sources X and Y, with respect to a fidelity criterion. They have established the rate-distortion function $R*_{X|Y}(D)$ for the case where the side information Y is perfectly known to the decoder only. For a given target distortion D, $R*_{X|Y}(D)$ in general verifies $R_{X|Y}(D) \leq R*_{X|Y}(D) \leq R_X(D)$, where $R_{X|Y}(D)$ is the rate required to encode X if Y is available to both the encoder and the decoder, and R_X is the minimal rate for encoding X without SI. These results give achievable rate bounds, however the design of codes and practical solutions for compression and communication applications remain a widely open issue.

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SMIS Project-Team

3. Research Program

3.1. Embedded Data Management

The challenge tackled is this research action is twofold: (1) to design embedded database techniques matching the hardware constraints of (current and future) smart objects and (2) to set up co-design rules helping hardware manufacturers to calibrate their future platforms to match the requirements of data driven applications. While a large body of work has been conducted on data management techniques for high-end servers (storage, indexation and query optimization models minimizing the I/O bottleneck, parallel DBMS, main memory DBMS, etc.), less research efforts have been placed on embedded database techniques. Light versions of popular DBMS have been designed for powerful handheld devices; yet DBMS vendors have never addressed the complex problem of embedding database components into chips. Proposals dedicated to databases embedded on chip usually consider small databases, stored in the non-volatile memory of the microcontroller –hundreds of kilobytes– and rely on NOR Flash or EEPROM technologies. Conversely, SMIS is pioneering the combination of microcontrollers and NAND Flash constraints to manage Gigabyte(s) size embedded databases. We present below the positioning of SMIS with respect to international teams conducting research on topics which may be connected to the addressed problem, namely work on electronic stable storage, RAM consumption and specific hardware platforms.

Major database teams are investigating data management issues related to hardware advances (EPFL: A. Ailamaki, CWI: M. Kersten, U. Of Wisconsin: J. M. Patel, Columbia: K. Ross, UCSB: A. El Abbadi, IBM Almaden: C. Mohan, etc.). While there are obvious links with our research on embedded databases, these teams target high-end computers and do not consider highly constrained architectures with non traditional hardware resources balance. At the other extreme, sensors (ultra-light computing devices) are considered by several research teams (e.g., UC Berkeley: D. Culler, ITU: P. Bonnet, Johns Hopkins University: A. Terzis, MIT: S. Madden, etc.). The focus is on the processing of continuous streams of collected data. Although the devices we consider share some hardware constraints with sensors, the objectives of both environments strongly diverge in terms of data cardinality and complexity, query complexity and data confidentiality requirements. Several teams are looking at efficient indexes on flash (HP LABS: G. Graefe, U. Minnesota: B. Debnath, U. Massachusetts: Y. Diao, Microsoft: S. Nath, etc.). Some studies try to minimize the RAM consumption, but the considered RAM/stable storage ratio is quite large compared to the constraints of the embedded context. Finally, a large number of teams have focused on the impact of flash memory on database system design (we presented an exhaustive state of the art in a VLDB tutorial [34]). The work conducted in the SMIS team on bi-modal flash devices takes the opposite direction, proposing to influence the design of flash devices by the expression of database requirements instead of running after the constantly evolving flash device technology.

3.2. Access and Usage Control Models

Access control management has been deeply studied for decades. Different models have been proposed to declare and administer access control policies, like DAC, MAC, RBAC, TMAC, and OrBAC. While access control management is well established, new models are being defined to cope with privacy requirements. Privacy management distinguishes itself from traditional access control is the sense that the data to be protected is personal. Hence, the user's consent must be reflected in the access control policies, as well as the usage of the data, its collection rules and its retention period, which are principles safeguarded by law and must be controlled carefully.

The research community working on privacy models is broad, and involves many teams worldwide including in France ENST-B, LIRIS, Inria LICIT, and LRI, and at the international level IBM Almaden, Purdue Univ., Politecnico di Milano and Univ. of Milano, George Mason Univ., Univ. of Massachusetts, Univ. of Texas and Colorado State Univ. to cite a few. Pioneer attempts towards privacy wary systems include the P3P Platform for Privacy Preservation [36] and Hippocratic databases [29]. In the last years, many other policy languages have been proposed for different application scenarios, including EPAL [40], XACML [39] and WSPL [32]. Hippocratic databases are inspired by the axiom that databases should be responsible for the privacy preservation of the data they manage. The architecture of a Hippocratic database is based on ten guiding principles derived from privacy laws.

The trend worldwide has been to propose enhanced access control policies to capture finer behavior and bridge the gap with privacy policies. To cite a few, Ardagna *et al.* (Univ. Milano) enables actions to be performed after data collection (like notification or removal), purpose binding features have been studied by Lefevre *et al.* (IBM Almaden), and Ni *et al.* (Purdue Univ.) have proposed obligations and have extended the widely used RBAC model to support privacy policies.

The positioning of the SMIS team within this broad area is rather (1) to focus on intuitive or automatic tools helping the individual to control some facets of her privacy (e.g., data retention, minimal collection) instead of increasing the expressiveness but also the complexity of privacy models and (2) to push concrete models enriched by real-case (e.g., medical) scenarios and by a joint work with researchers in Law.

3.3. Tamper-resistant Data Management

Tamper-resistance refers to the capacity of a system to defeat confidentiality and integrity attacks. This problem is complementary to access control management while being (mostly) orthogonal to the way access control policies are defined. Security surveys regularly point out the vulnerability of database servers against external (i.e., by intruders) and internal (i.e., by employees) attacks. Several attempts have been made in commercial DBMSs to strengthen server-based security, e.g., by separating the duty between DBA and DSA (Data Security Administrator), by encrypting the database footprint and by securing the cryptographic material using Hardware Security Modules (HSM) [35]. To face internal attacks, client-based security approaches have been investigated where the data is stored encrypted on the server and is decrypted only on the client side. Several contributions have been made in this direction, notably by U. of California Irvine (S. Mehrotra, Database Service Provider model), IBM Almaden (R. Agrawal, computation on encrypted data), U. of Milano (E. Damiani, encryption schemes), Purdue U. (E. Bertino, XML secure publication), U. of Washington (D. Suciu, provisional access) to cite a few seminal works. An alternative, recently promoted by Stony Brook Univ. (R. Sion), is to augment the security of the server by associating it with a tamper-resistant hardware module in charge of the security aspects. Contrary to traditional HSM, this module takes part in the query computation and performs all data decryption operations. SMIS investigates another direction based on the use of a tamper-resistant hardware module on the client side. Most of our contributions in this area are based on exploiting the tamper-resistance of secure tokens to build new data protection schemes.

While our work on Privacy-Preserving data Publishing (PPDP) is still related to tamper-resistance, a complementary positioning is required for this specific topic. The primary goal of PPDP is to anonymize/sanitize microdata sets before publishing them to serve statistical analysis purposes. PPDP (and privacy in databases in general) is a hot topic since 2000, when it was introduced by IBM Research (IBM Almaden: R. Agrawal, IBM Watson: C.C. Aggarwal), and many teams, mostly north American universities or research centres, study this topic (e.g., PORTIA DB-Privacy project regrouping universities such as Stanford with H. Garcia-Molina). Much effort has been devoted by the scientific community to the definition of privacy models exhibiting better privacy guarantees or better utility or a balance of both (such as differential privacy studied by C. Dwork: Microsoft Research or D. Kifer: Penn-State Univ and J. Gehrke: Cornell Univ) and thorough surveys exist that provide a large overview of existing PPDP models and mechanisms [37]. These works are however orthogonal to our approach in that they make the hypothesis of a trustworthy central server that can execute the anonymization process. In our work, this is not the case. We consider an architecture composed of a large population of tamper-resistant devices weakly connected to an untrusted infrastructure and study how to compute

PPDP problems in this context [1]. Hence, our work has some connections with the works done on Privacy Preserving Data Collection (Stevens Institute of Tech. / Rutgers Univ,NJ: R.N.Wright, Univ Austin Texas: V. Shmatikov), on Secure Multi-party Computing for Privacy Preserving Data Mining (Rutgers Univ: J. Vaidya, Purdue Univ: C. Clifton) and on distributed PPDP algorithms (Univ Wisconsin: D. DeWitt, Univ Michigan: K. Lefevre, Rutgers Univ: J. Vaidya, Purdue Univ: C. Clifton) while none of them share the same architectural hypothesis as us.

STARS Project-Team

3. Research Program

3.1. Introduction

Stars follows three main research directions: perception for activity recognition, semantic activity recognition, and software engineering for activity recognition. **These three research directions are interleaved**: *the software engineering* research direction provides new methodologies for building safe activity recognition systems and *the perception* and *the semantic activity recognition* directions provide new activity recognition techniques which are designed and validated for concrete video analytic and healthcare applications. Conversely, these concrete systems raise new software issues that enrich the software engineering research direction.

Transversely, we consider a *new research axis in machine learning*, combining a priori knowledge and learning techniques, to set up the various models of an activity recognition system. A major objective is to automate model building or model enrichment at the perception level and at the understanding level.

3.2. Perception for Activity Recognition

Participants: François Brémond, Sabine Moisan, Monique Thonnat.

Computer Vision; Cognitive Systems; Learning; Activity Recognition.

3.2.1. Introduction

Our main goal in perception is to develop vision algorithms able to address the large variety of conditions characterizing real world scenes in terms of sensor conditions, hardware requirements, lighting conditions, physical objects, and application objectives. We have also several issues related to perception which combine machine learning and perception techniques: learning people appearance, parameters for system control and shape statistics.

3.2.2. Appearance Models and People Tracking

An important issue is to detect in real-time physical objects from perceptual features and predefined 3D models. It requires finding a good balance between efficient methods and precise spatio-temporal models. Many improvements and analysis need to be performed in order to tackle the large range of people detection scenarios.

Appearance models. In particular, we study the temporal variation of the features characterizing the appearance of a human. This task could be achieved by clustering potential candidates depending on their position and their reliability. This task can provide any people tracking algorithms with reliable features allowing for instance to (1) better track people or their body parts during occlusion, or to (2) model people appearance for re-identification purposes in mono and multi-camera networks, which is still an open issue. The underlying challenge of the person re-identification problem arises from significant differences in illumination, pose and camera parameters. The re-identification approaches have two aspects: (1) establishing correspondences between body parts and (2) generating signatures that are invariant to different color responses. As we have already several descriptors which are color invariant, we now focus more on aligning two people detection and on finding their corresponding body parts. Having detected body parts, the approach can handle pose variations. Further, different body parts might have different influence on finding the correct match among a whole gallery dataset. Thus, the re-identification approaches have to search for matching strategies. As the results of the re-identification are always given as the ranking list, re-identification focuses on learning to rank. "Learning to rank" is a type of machine learning problem, in which the goal is to automatically construct a ranking model from a training data.

Therefore, we work on information fusion to handle perceptual features coming from various sensors (several cameras covering a large scale area or heterogeneous sensors capturing more or less precise and rich information). New 3D RGB-D sensors are also investigated, to help in getting an accurate segmentation for specific scene conditions.

Long term tracking. For activity recognition we need robust and coherent object tracking over long periods of time (often several hours in videosurveillance and several days in healthcare). To guarantee the long term coherence of tracked objects, spatio-temporal reasoning is required. Modeling and managing the uncertainty of these processes is also an open issue. In Stars we propose to add a reasoning layer to a classical Bayesian framework modeling the uncertainty of the tracked objects. This reasoning layer can take into account the a priori knowledge of the scene for outlier elimination and long-term coherency checking.

Controlling system parameters. Another research direction is to manage a library of video processing programs. We are building a perception library by selecting robust algorithms for feature extraction, by insuring they work efficiently with real time constraints and by formalizing their conditions of use within a program supervision model. In the case of video cameras, at least two problems are still open: robust image segmentation and meaningful feature extraction. For these issues, we are developing new learning techniques.

3.3. Semantic Activity Recognition

Participants: François Brémond, Sabine Moisan, Monique Thonnat.

Activity Recognition, Scene Understanding, Computer Vision

3.3.1. Introduction

Semantic activity recognition is a complex process where information is abstracted through four levels: signal (e.g. pixel, sound), perceptual features, physical objects and activities. The signal and the feature levels are characterized by strong noise, ambiguous, corrupted and missing data. The whole process of scene understanding consists in analyzing this information to bring forth pertinent insight of the scene and its dynamics while handling the low level noise. Moreover, to obtain a semantic abstraction, building activity models is a crucial point. A still open issue consists in determining whether these models should be given a priori or learned. Another challenge consists in organizing this knowledge in order to capitalize experience, share it with others and update it along with experimentation. To face this challenge, tools in knowledge engineering such as machine learning or ontology are needed.

Thus we work along the following research axes: high level understanding (to recognize the activities of physical objects based on high level activity models), learning (how to learn the models needed for activity recognition) and activity recognition and discrete event systems.

3.3.2. High Level Understanding

A challenging research axis is to recognize subjective activities of physical objects (i.e. human beings, animals, vehicles) based on a priori models and objective perceptual measures (e.g. robust and coherent object tracks).

To reach this goal, we have defined original activity recognition algorithms and activity models. Activity recognition algorithms include the computation of spatio-temporal relationships between physical objects. All the possible relationships may correspond to activities of interest and all have to be explored in an efficient way. The variety of these activities, generally called video events, is huge and depends on their spatial and temporal granularity, on the number of physical objects involved in the events, and on the event complexity (number of components constituting the event).

Concerning the modeling of activities, we are working towards two directions: the uncertainty management for representing probability distributions and knowledge acquisition facilities based on ontological engineering techniques. For the first direction, we are investigating classical statistical techniques and logical approaches. For the second direction, we built a language for video event modeling and a visual concept ontology (including color, texture and spatial concepts) to be extended with temporal concepts (motion, trajectories, events ...) and other perceptual concepts (physiological sensor concepts ...).

3.3.3. Learning for Activity Recognition

Given the difficulty of building an activity recognition system with a priori knowledge for a new application, we study how machine learning techniques can automate building or completing models at the perception level and at the understanding level.

At the understanding level, we are learning primitive event detectors. This can be done for example by learning visual concept detectors using SVMs (Support Vector Machines) with perceptual feature samples. An open question is how far can we go in weakly supervised learning for each type of perceptual concept (i.e. leveraging the human annotation task). A second direction is to learn typical composite event models for frequent activities using trajectory clustering or data mining techniques. We name composite event a particular combination of several primitive events.

3.3.4. Activity Recognition and Discrete Event Systems

The previous research axes are unavoidable to cope with the semantic interpretations. However they tend to let aside the pure event driven aspects of scenario recognition. These aspects have been studied for a long time at a theoretical level and led to methods and tools that may bring extra value to activity recognition, the most important being the possibility of formal analysis, verification and validation.

We have thus started to specify a formal model to define, analyze, simulate, and prove scenarios. This model deals with both absolute time (to be realistic and efficient in the analysis phase) and logical time (to benefit from well-known mathematical models providing re-usability, easy extension, and verification). Our purpose is to offer a generic tool to express and recognize activities associated with a concrete language to specify activities in the form of a set of scenarios with temporal constraints. The theoretical foundations and the tools being shared with Software Engineering aspects, they will be detailed in section 3.4 .

The results of the research performed in perception and semantic activity recognition (first and second research directions) produce new techniques for scene understanding and contribute to specify the needs for new software architectures (third research direction).

3.4. Software Engineering for Activity Recognition

Participants: Sabine Moisan, Annie Ressouche, Jean-Paul Rigault, François Brémond.

Software Engineering, Generic Components, Knowledge-based Systems, Software Component Platform, Object-oriented Frameworks, Software Reuse, Model-driven Engineering

The aim of this research axis is to build general solutions and tools to develop systems dedicated to activity recognition. For this, we rely on state-of-the art Software Engineering practices to ensure both sound design and easy use, providing genericity, modularity, adaptability, reusability, extensibility, dependability, and maintainability.

This research requires theoretical studies combined with validation based on concrete experiments conducted in Stars. We work on the following three research axes: *models* (adapted to the activity recognition domain), *platform architecture* (to cope with deployment constraints and run time adaptation), and *system verification* (to generate dependable systems). For all these tasks we follow state of the art Software Engineering practices and, if needed, we attempt to set up new ones.

3.4.1. Platform Architecture for Activity Recognition

In the former project teams Orion and Pulsar, we have developed two platforms, one (VSIP), a library of real-time video understanding modules and another one, LAMA [14], a software platform enabling to design not only knowledge bases, but also inference engines, and additional tools. LAMA offers toolkits to build and to adapt all the software elements that compose a knowledge-based system.

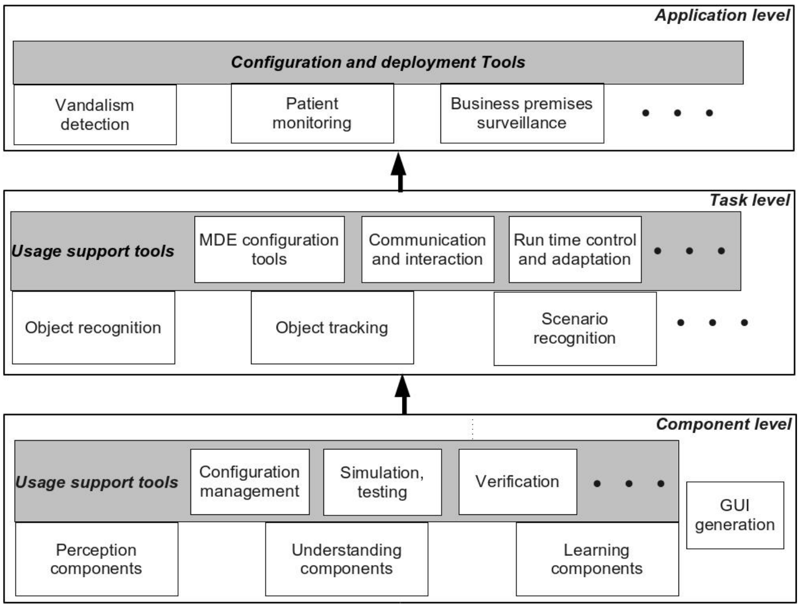

Figure 4. Global Architecture of an Activity Recognition The gray areas contain software engineering support modules whereas the other modules correspond to software components (at Task and Component levels) or to generated systems (at Application level).

Figure 4 presents our conceptual vision for the architecture of an activity recognition platform. It consists of three levels:

- The **Component Level**, the lowest one, offers software components providing elementary operations and data for perception, understanding, and learning.
  - *Perception components* contain algorithms for sensor management, image and signal analysis, image and video processing (segmentation, tracking...), etc.
  - *Understanding components* provide the building blocks for Knowledge-based Systems: knowledge representation and management, elements for controlling inference engine strategies, etc.
  - *Learning components* implement different learning strategies, such as Support Vector Machines (SVM), Case-based Learning (CBL), clustering, etc.

  An Activity Recognition system is likely to pick components from these three packages. Hence, tools must be provided to configure (select, assemble), simulate, verify the resulting component combination. Other support tools may help to generate task or application dedicated languages or graphic interfaces.

- The **Task Level**, the middle one, contains executable realizations of individual tasks that will collaborate in a particular final application. Of course, the code of these tasks is built on top of the components from the previous level. We have already identified several of these important tasks: Object Recognition, Tracking, Scenario Recognition... In the future, other tasks will probably enrich this level.

  For these tasks to nicely collaborate, communication and interaction facilities are needed. We shall also add MDE-enhanced tools for configuration and run-time adaptation.

- The **Application Level** integrates several of these tasks to build a system for a particular type of application, e.g., vandalism detection, patient monitoring, aircraft loading/unloading surveillance, etc.. Each system is parameterized to adapt to its local environment (number, type, location of sensors, scene geometry, visual parameters, number of objects of interest...). Thus configuration and deployment facilities are required.

The philosophy of this architecture is to offer at each level a balance between the widest possible genericity and the maximum effective reusability, in particular at the code level.

To cope with real application requirements, we shall also investigate distributed architecture, real time implementation, and user interfaces.

Concerning implementation issues, we shall use when possible existing open standard tools such as NuSMV for model-checking, Eclipse for graphic interfaces or model engineering support, Alloy for constraint representation and SAT solving for verification, etc. Note that, in Figure 4 , some of the boxes can be naturally adapted from SUP existing elements (many perception and understanding components, program supervision, scenario recognition...) whereas others are to be developed, completely or partially (learning components, most support and configuration tools).

3.4.2. Discrete Event Models of Activities

As mentioned in the previous section (3.3) we have started to specify a formal model of scenario dealing with both absolute time and logical time. Our scenario and time models as well as the platform verification tools rely on a formal basis, namely the synchronous paradigm. To recognize scenarios, we consider activity descriptions as synchronous reactive systems and we apply general modeling methods to express scenario behavior.

Activity recognition systems usually exhibit many safeness issues. From the software engineering point of view we only consider software security. Our previous work on verification and validation has to be pursued; in particular, we need to test its scalability and to develop associated tools. Model-checking is an appealing technique since it can be automatized and helps to produce a code that has been formally proved. Our verification method follows a compositional approach, a well-known way to cope with scalability problems in model-checking.

Moreover, recognizing real scenarios is not a purely deterministic process. Sensor performance, precision of image analysis, scenario descriptions may induce various kinds of uncertainty. While taking into account this uncertainty, we should still keep our model of time deterministic, modular, and formally verifiable. To formally describe probabilistic timed systems, the most popular approach involves probabilistic extension of timed automata. New model checking techniques can be used as verification means, but relying on model checking techniques is not sufficient. Model checking is a powerful tool to prove decidable properties but introducing uncertainty may lead to infinite state or even undecidable properties. Thus model checking validation has to be completed with non exhaustive methods such as abstract interpretation.

3.4.3. Model-Driven Engineering for Configuration and Control and Control of Video Surveillance systems

Model-driven engineering techniques can support the configuration and dynamic adaptation of video surveillance systems designed with our SUP activity recognition platform. The challenge is to cope with the many—functional as well as nonfunctional—causes of variability both in the video application specification and in the concrete SUP implementation. We have used *feature models* to define two models: a generic model of video surveillance applications and a model of configuration for SUP components and chains. Both of them express variability factors. Ultimately, we wish to automatically generate a SUP component assembly from an application specification, using models to represent transformations [45]. Our models are enriched with intra- and inter-models constraints. Inter-models constraints specify models to represent transformations. Feature models are appropriate to describe variants; they are simple enough for video surveillance experts to express their requirements. Yet, they are powerful enough to be liable to static analysis [77]. In particular, the constraints can be analyzed as a SAT problem.

An additional challenge is to manage the possible run-time changes of implementation due to context variations (e.g., lighting conditions, changes in the reference scene, etc.). Video surveillance systems have to dynamically adapt to a changing environment. The use of models at run-time is a solution. We are defining adaptation rules corresponding to the dependency constraints between specification elements in one model and software variants in the other [44], [89], [82].

THOTH Project-Team

3. Research Program

3.1. Designing and learning structured models

The task of understanding image and video content has been interpreted in several ways over the past few decades, namely image classification, detecting objects in a scene, recognizing objects and their spatial extents in an image, estimating human poses, recovering scene geometry, recognizing activities performed by humans. However, addressing all these problems individually provides us with a partial understanding of the scene at best, leaving much of the visual data unexplained.

One of the main goals of this research axis is to go beyond the initial attempts that consider only a subset of tasks jointly, by developing novel models for a more complete understanding of scenes to address all the component tasks. We propose to incorporate the structure in image and video data explicitly into the models. In other words, our models aim to satisfy the complex sets of constraints that exist in natural images and videos. Examples of such constraints include: (i) relations between objects, like signs for shops indicate the presence of buildings, people on a road are usually walking or standing, (ii) higher-level semantic relations involving the type of scene, geographic location, and the plausible actions as a global constraint, e.g., an image taken at a swimming pool is unlikely to contain cars, (iii) relating objects occluded in some of the video frames to content in other frames, where they are more clearly visible as the camera or the object itself move, with the use of long-term trajectories and video object proposals.

This research axis will focus on three topics. The first is developing deep features for video. This involves designing rich features available in the form of long-range temporal interactions among pixels in a video sequence to learn a representation that is truly spatio-temporal in nature. The focus of the second topic is the challenging problem of modeling human activities in video, starting from human activity descriptors to building intermediate spatio-temporal representations of videos, and then learning the interactions among humans, objects and scenes temporally. The last topic is aimed at learning models that capture the relationships among several objects and regions in a single image scene, and additionally, among scenes in the case of an image collection or a video. The main scientific challenges in this topic stem from learning the structure of the probabilistic graphical model as well as the parameters of the cost functions quantifying the relationships among its entities. In the following we will present work related to all these three topics and then elaborate on our research directions.

- **Deep features for vision.** Deep learning models provide a rich representation of complex objects but in return have a large number of parameters. Thus, to work well on difficult tasks, a large amount of data is required. In this context, video presents several advantages: objects are observed from a large range of viewpoints, motion information allows the extraction of moving objects and parts, and objects can be differentiated by their motion patterns. We initially plan to develop deep features for videos that incorporate temporal information at multiple scales. We then plan to further exploit the rich content in video by incorporating additional cues, such as the detection of people and their body-joint locations in video, minimal prior knowledge of the object of interest, with the goal of learning a representation that is more appropriate for video understanding. In other words, a representation that is learned from video data and targeted at specific applications. For the application of recognizing human activities, this involves learning deep features for humans and their body-parts with all their spatiotemporal variations, either directly from raw video data or “pre-processed” videos containing human detections. For the application of object tracking, this task amounts to learning object-specific deep representations, further exploiting the limited annotation provided to identify the object.
- **Modeling human activities in videos.** Humans and their activities are not only one of the most frequent and interesting subjects in videos but also one of the hardest to analyze owing to the

complexity of the human form, clothing and movements. As part of this task, the Thoth project-team plans to build on state-of-the-art approaches for spatio-temporal representation of videos. This will involve using the dominant motion in the scene as well as the local motion of individual parts undergoing a rigid motion. Such motion information also helps in reasoning occlusion relationships among people and objects, and the state of the object. This novel spatio-temporal representation ultimately provides the equivalent of object proposals for videos, and is an important component for learning algorithms using minimal supervision. To take this representation even further, we aim to integrate the proposals and the occlusion relationships with methods for estimating human pose in videos, thus leveraging the interplay among body-joint locations, objects in the scene, and the activity being performed. For example, the locations of shoulder, elbow and wrist of a person drinking coffee are constrained to move in a certain way, which is completely different from the movement observed when a person is typing. In essence, this step will model human activities by dynamics in terms of both low-level movements of body-joint locations and global high-level motion in the scene.

- **Structured models.** The interactions among various elements in a scene, such as, the objects and regions in it, the motion of object parts or entire objects themselves, form a key element for understanding image or video content. These rich cues define the structure of visual data and how it evolves spatio-temporally. We plan to develop a novel graphical model to exploit this structure. The main components in this graphical model are spatio-temporal regions (in the case of video or simply image regions), which can represent object parts or entire objects themselves, and the interactions among several entities. The dependencies among the scene entities are defined with a higher order or a global cost function. A higher order constraint is a generalization of the pairwise interaction term, and is a cost function involving more than two components in the scene, e.g., several regions, whereas a global constraint imposes a cost term over the entire image or video, e.g., a prior on the number of people expected in the scene. The constraints we plan to include generalize several existing methods, which are limited to pairwise interactions or a small restrictive set of higher-order costs. In addition to learning the parameters of these novel functions, we will focus on learning the structure of the graph itself—a challenging problem that is seldom addressed in current approaches. This provides an elegant way to go beyond state-of-the-art deep learning methods, which are limited to learning the high-level interaction among parts of an object, by learning the relationships among objects.

3.2. Learning of visual models from minimal supervision

Today's approaches to visual recognition learn models for a limited and fixed set of visual categories with fully supervised classification techniques. This paradigm has been adopted in the early 2000's, and within it enormous progress has been made over the last decade.

The scale and diversity in today's large and growing image and video collections (such as, e.g., broadcast archives, and personal image/video collections) call for a departure from the current paradigm. This is the case because to answer queries about such data, it is unfeasible to learn the models of visual content by manually and precisely annotating every relevant concept, object, scene, or action category in a representative sample of everyday conditions. For one, it will be difficult, or even impossible to decide a-priori what are the relevant categories and the proper granularity level. Moreover, the cost of such annotations would be prohibitive in most application scenarios. One of the main goals of the Thoth project-team is to develop a new framework for learning visual recognition models by actively exploring large digital image and video sources (off-line archives as well as growing on-line content), and exploiting the weak supervisory signal provided by the accompanying metadata (such as captions, keywords, tags, subtitles, or scripts) and audio signal (from which we can for example extract speech transcripts, or exploit speaker recognition models).

Textual metadata has traditionally been used to index and search for visual content. The information in metadata is, however, typically sparse (e.g., the location and overall topic of newscasts in a video archive [0])

[0] For example at the Dutch national broadcast archive Netherlands Institute of Sound and Vision, with whom we collaborated in the EU FP7 project AXES, typically one or two sentences are used in the metadata to describe a one hour long TV program.

and noisy (e.g., a movie script may tell us that two persons kiss in some scene, but not when, and the kiss may occur off screen or not have survived the final cut). For this reason, metadata search should be complemented by visual content based search, where visual recognition models are used to localize content of interest that is not mentioned in the metadata, to increase the usability and value of image/video archives. *The key insight that we build on in this research axis is that while the metadata for a single image or video is too sparse and noisy to rely on for search, the metadata associated with large video and image databases collectively provide an extremely versatile source of information to learn visual recognition models.* This form of "embedded annotation" is rich, diverse and abundantly available. Mining these correspondences from the web, TV and film archives, and online consumer generated content sites such as Flickr, Facebook, or YouTube, guarantees that the learned models are representative for many different situations, unlike models learned from manually collected fully supervised training data sets which are often biased.

The approach we propose to address the limitations of the fully supervised learning paradigm aligns with "Big Data" approaches developed in other areas: we rely on the orders-of-magnitude-larger training sets that have recently become available with metadata to compensate for less explicit forms of supervision. This will form a sustainable approach to learn visual recognition models for a much larger set of categories with little or no manual intervention. Reducing and ultimately removing the dependency on manual annotations will dramatically reduce the cost of learning visual recognition models. This in turn will allow such models to be used in many more applications, and enable new applications based on visual recognition beyond a fixed set of categories, such as natural language based querying for visual content. This is an ambitious goal, given the sheer volume and intrinsic variability of the every day visual content available on-line, and the lack of a universally accepted formalism for modeling it. Yet, the potential payoff is a breakthrough in visual object recognition and scene understanding capabilities.

This research axis is organized into the following three sub-tasks:

- **Weakly supervised learning.** For object localization we will go beyond current methods that learn one category model at a time and develop methods that learn models for different categories concurrently. This allows "explaining away" effects to be leveraged, i.e., if a certain region in an image has been identified as an instance of one category, it cannot be an instance of another category at the same time. For weakly supervised detection in video we will consider detection proposal methods. While these are effective for still images, recent approaches for the spatio-temporal domain need further improvements to be similarly effective. Furthermore, we will exploit appearance and motion information jointly over a set of videos. In the video domain we will also continue to work on learning recognition models from subtitle and script information. The basis of leveraging the script data which does not have a temporal alignment with the video, is to use matches in the narrative in the script and the subtitles (which do have a temporal alignment with the video). We will go beyond simple correspondences between names and verbs relating to self-motion, and match more complex sentences related to interaction with objects and other people. To deal with the limited amount of occurrences of such actions in a single movie, we will consider approaches that learn action models across a collection of movies.
- **Online learning of visual models.** As a larger number of visual category models is being learned, online learning methods become important, since new training data and categories will arrive over time. We will develop online learning methods that can incorporate new examples for existing category models, and learn new category models from few examples by leveraging similarity to related categories using multi-task learning methods. Here we will develop new distance-based classifiers and attribute and label embedding techniques, and explore the use of NLP techniques such as skipgram models to automatically determine between which classes transfer should occur. Moreover, NLP will be useful in the context of learning models for many categories to identify synonyms, and to determine cases of polysemy (e.g. jaguar car brand v.s. jaguar animal), and merge or refine categories accordingly. Ultimately this will result in methods that are able to learn an"encyclopedia" of visual models.
- **Visual search from unstructured textual queries.** We will build on recent approaches that learn

recognition models on-the-fly (as the query is issued) from generic image search engines such as Google Images. While it is feasible to learn models in this manner in a matter of seconds, it is challenging to use the model to retrieve relevant content in real-time from large video archives of more than a few thousand hours. To achieve this requires feature compression techniques to store visual representations in memory, and cascaded search techniques to avoid exhaustive search. This approach, however, leaves untouched the core problem of how to associate visual material with the textual query in the first place. The second approach we will explore is based on image annotation models. In particular we will go beyond image-text retrieval methods by using recurrent neural networks such as Elman networks or long short-term memory (LSTM) networks to generate natural language sentences to describe images.

3.3. Large-scale learning and optimization

We have entered an era of massive data acquisition, leading to the revival of an old scientific utopia: it should be possible to better understand the world by automatically converting data into knowledge. It is also leading to a new economic paradigm, where data is a valuable asset and a source of activity. Therefore, developing scalable technology to make sense of massive data has become a strategic issue. Computer vision has already started to adapt to these changes.

In particular, very high dimensional models such as deep networks are becoming highly popular and successful for visual recognition. This change is closely related to the advent of big data. On the one hand, these models involve a huge number of parameters and are rich enough to represent well complex objects such as natural images or text corpora. On the other hand, they are prone to overfitting (fitting too closely to training data without being able to generalize to new unseen data) despite regularization; to work well on difficult tasks, they require a large amount of labelled data that has been available only recently. Other cues may explain their success: the deep learning community has made significant engineering efforts, making it possible to learn in a day on a GPU large models that would have required weeks of computations on a traditional CPU, and it has accumulated enough empirical experience to find good hyper-parameters for its networks.

To learn the huge number of parameters of deep hierarchical models requires scalable optimization techniques and large amounts of data to prevent overfitting. This immediately raises two major challenges: how to learn without large amounts of labeled data, or with weakly supervised annotations? How to efficiently learn such huge-dimensional models? To answer the above challenges, we will concentrate on the design and theoretical justifications of deep architectures including our recently proposed deep kernel machines, with a focus on weakly supervised and unsupervised learning, and develop continuous and discrete optimization techniques that push the state of the art in terms of speed and scalability.

This research axis will be developed into three sub-tasks:

- **Deep kernel machines for structured data.** Deep kernel machines combine advantages of kernel methods and deep learning. Both approaches rely on high-dimensional models. Kernels implicitly operate in a space of possibly infinite dimension, whereas deep networks explicitly construct high-dimensional nonlinear data representations. Yet, these approaches are complementary: Kernels can be built with deep learning principles such as hierarchies and convolutions, and approximated by multilayer neural networks. Furthermore, kernels work with structured data and have well understood theoretical principles. Thus, a goal of the Thoth project-team is to design and optimize the training of such deep kernel machines.
- **Large-scale parallel optimization.** Deep kernel machines produce nonlinear representations of input data points. After encoding these data points, a learning task is often formulated as a *large-scale convex optimization problem*; for example, this is the case for linear support vector machines, logistic regression classifiers, or more generally many empirical risk minimization formulations. We intend to pursue recent efforts for making convex optimization techniques that are dedicated to machine learning more scalable. Most existing approaches address scalability issues either in model size (meaning that the function to minimize is defined on a domain of very high dimension), or in the amount of training data (typically, the objective is a large sum of elementary functions). There is

thus a large room for improvements for techniques that jointly take these two criteria into account.

- **Large-scale graphical models.** To represent structured data, we will also investigate graphical models and their optimization. The challenge here is two-fold: designing an adequate cost function and minimizing it. While several cost functions are possible, their utility will be largely determined by the efficiency and the effectiveness of the optimization algorithms for solving them. It is a combinatorial optimization problem involving billions of variables and is NP-hard in general, requiring us to go beyond the classical approximate inference techniques. The main challenges in minimizing cost functions stem from the large number of variables to be inferred, the inherent structure of the graph induced by the interaction terms (e.g., pairwise terms), and the high-arity terms which constrain multiple entities in a graph.

3.4. Datasets and evaluation

Standard benchmarks with associated evaluation measures are becoming increasingly important in computer vision, as they enable an objective comparison of state-of-the-art approaches. Such datasets need to be relevant for real-world application scenarios; challenging for state-of-the-art algorithms; and large enough to produce statistically significant results.

A decade ago, small datasets were used to evaluate relatively simple tasks, such as for example interest point matching and detection. Since then, the size of the datasets and the complexity of the tasks gradually evolved. An example is the Pascal Visual Object Challenge with 20 classes and approximately 10,000 images, which evaluates object classification and detection. Another example is the ImageNet challenge, including thousands of classes and millions of images. In the context of video classification, the TrecVid Multimedia Event Detection challenges, organized by NIST, evaluate activity classification on a dataset of over 200,000 video clips, representing more than 8,000 hours of video, which amounts to 11 months of continuous video.

Almost all of the existing image and video datasets are annotated by hand; it is the case for all of the above cited examples. In some cases, they present limited and unrealistic viewing conditions. For example, many images of the ImageNet dataset depict upright objects with virtually no background clutter, and they may not capture particularly relevant visual concepts: most people would not know the majority of subcategories of snakes cataloged in ImageNet. This holds true for video datasets as well, where in addition a taxonomy of action and event categories is missing.

Our effort on data collection and evaluation will focus on two directions. First, we will design and assemble video datasets, in particular for action and activity recognition. This includes defining relevant taxonomies of actions and activities. Second, we will provide data and define evaluation protocols for weakly supervised learning methods. This does not mean of course that we will forsake human supervision altogether: some amount of ground-truth labeling is necessary for experimental validation and comparison to the state of the art. Particular attention will be payed to the design of efficient annotation tools.

Not only do we plan to collect datasets, but also to provide them to the community, together with accompanying evaluation protocols and software, to enable a comparison of competing approaches for action recognition and large-scale weakly supervised learning. Furthermore, we plan to set up evaluation servers together with leader-boards, to establish an unbiased state of the art on held out test data for which the ground-truth annotations are not distributed. This is crucial to avoid tuning the parameters for a specific dataset and to guarantee a fair evaluation.

- **Action recognition.** We will develop datasets for recognizing human actions and human-object interactions (including multiple persons) with a significant number of actions. Almost all of today's action recognition datasets evaluate classification of short video clips into a number of predefined categories, in many cases a number of different sports, which are relatively easy to identify by their characteristic motion and context. However, in many real-world applications the goal is to identify and localize actions in entire videos, such as movies or surveillance videos of several hours. The actions targeted here are "real-world" and will be defined by compositions of atomic actions into higher-level activities. One essential component is the definition of relevant taxonomies of actions and activities. We think that such a definition needs to rely on a decomposition of actions into poses, objects and scenes, as determining all possible actions without such a decomposition is not feasible. We plan to provide annotations for spatio-temporal localization of humans as well as relevant objects and scene parts for a large number of actions and videos.

- **Weakly supervised learning.** We will collect weakly labeled images and videos for training. The collection process will be semi-automatic. We will use image or video search engines such as Google Image Search, Flickr or YouTube to find visual data corresponding to the labels. Initial datasets will be obtained by manually correcting whole-image/video labels, i.e., the approach will evaluate how well the object model can be learned if the entire image or video is labeled, but the object model has to be extracted automatically. Subsequent datasets will features noisy and incorrect labels. Testing will be performed on PASCAL VOC'07 and ImageNet, but also on more realistic datasets similar to those used for training, which we develop and manually annotate for evaluation. Our dataset will include both images and videos, the categories represented will include objects, scenes as well as human activities, and the data will be presented in realistic conditions.
- **Joint learning from visual information and text.** Initially, we will use a selection from the large number of movies and TV series for which scripts are available on-line, see for example http://www.dailyscript.com and http://www.weeklyscript.com. These scripts can easily be aligned with the videos by establishing correspondences between script words and (timestamped) spoken ones obtained from the subtitles or audio track. The goal is to jointly learn from visual content and text. To measure the quality of such a joint learning, we will manually annotate some of the videos. Annotations will include the space-time locations of the actions as well as correct parsing of the sentence. While DVDs will, initially, receive most attention, we will also investigate the use of data obtained from web pages, for example images with captions, or images and videos surrounded by text. This data is by nature more noisy than scripts.

TITANE Project-Team

3. Research Program

3.1. Context

Geometric modeling and processing revolve around three main end goals: a computerized shape representation that can be visualized (creating a realistic or artistic depiction), simulated (anticipating the real) or realized (manufacturing a conceptual or engineering design). Aside from the mere editing of geometry, central research themes in geometric modeling involve conversions between physical (real), discrete (digital), and mathematical (abstract) representations. Going from physical to digital is referred to as shape acquisition and reconstruction; going from mathematical to discrete is referred to as shape approximation and mesh generation; going from discrete to physical is referred to as shape rationalization.

Geometric modeling has become an indispensable component for computational and reverse engineering. Simulations are now routinely performed on complex shapes issued not only from computer-aided design but also from an increasing amount of available measurements. The scale of acquired data is quickly growing: we no longer deal exclusively with individual shapes, but with entire *scenes*, possibly at the scale of entire cities, with many objects defined as structured shapes. We are witnessing a rapid evolution of the acquisition paradigms with an increasing variety of sensors and the development of community data, as well as disseminated data.

In recent years, the evolution of acquisition technologies and methods has translated in an increasing overlap of algorithms and data in the computer vision, image processing, and computer graphics communities. Beyond the rapid increase of resolution through technological advances of sensors and methods for mosaicing images, the line between laser scan data and photos is getting thinner. Combining, e.g., laser scanners with panoramic cameras leads to massive 3D point sets with color attributes. In addition, it is now possible to generate dense point sets not just from laser scanners but also from photogrammetry techniques when using a well-designed acquisition protocol. Depth cameras are getting increasingly common, and beyond retrieving depth information we can enrich the main acquisition systems with additional hardware to measure geometric information about the sensor and improve data registration: e.g., accelerometers or GPS for geographic location, and compasses or gyrometers for orientation. Finally, complex scenes can be observed at different scales ranging from satellite to pedestrian through aerial levels.

These evolutions allow practitioners to measure urban scenes at resolutions that were until now possible only at the scale of individual shapes. The related scientific challenge is however more than just dealing with massive data sets coming from increase of resolution, as complex scenes are composed of multiple objects with structural relationships. The latter relate i) to the way the individual shapes are grouped to form objects, object classes or hierarchies, ii) to geometry when dealing with similarity, regularity, parallelism or symmetry, and iii) to domain-specific semantic considerations. Beyond reconstruction and approximation, consolidation and synthesis of complex scenes require rich structural relationships.

The problems arising from these evolutions suggest that the strengths of geometry and images may be combined in the form of new methodological solutions such as photo-consistent reconstruction. In addition, the process of measuring the geometry of sensors (through gyrometers and accelerometers) often requires both geometry process and image analysis for improved accuracy and robustness. Modeling urban scenes from measurements illustrates this growing synergy, and it has become a central concern for a variety of applications ranging from urban planning to simulation through rendering and special effects.

3.2. Analysis

Complex scenes are usually composed of a large number of objects which may significantly differ in terms of complexity, diversity, and density. These objects must be identified and their structural relationships must be recovered in order to model the scenes with improved robustness, low complexity, variable levels of details and ultimately, semantization (automated process of increasing degree of semantic content).

Object classification is an ill-posed task in which the objects composing a scene are detected and recognized with respect to predefined classes, the objective going beyond scene segmentation. The high variability in each class may explain the success of the stochastic approach which is able to model widely variable classes. As it requires a priori knowledge this process is often domain-specific such as for urban scenes where we wish to distinguish between instances as ground, vegetation and buildings. Additional challenges arise when each class must be refined, such as roof super-structures for urban reconstruction.

Structure extraction consists in recovering structural relationships between objects or parts of object. The structure may be related to adjacencies between objects, hierarchical decomposition, singularities or canonical geometric relationships. It is crucial for effective geometric modeling through levels of details or hierarchical multiresolution modeling. Ideally we wish to learn the structural rules that govern the physical scene manufacturing. Understanding the main canonical geometric relationships between object parts involves detecting regular structures and equivalences under certain transformations such as parallelism, orthogonality and symmetry. Identifying structural and geometric repetitions or symmetries is relevant for dealing with missing data during data consolidation.

Data consolidation is a problem of growing interest for practitioners, with the increase of heterogeneous and defect-laden data. To be exploitable, such defect-laden data must be consolidated by improving the data sampling quality and by reinforcing the geometrical and structural relations sub-tending the observed scenes. Enforcing canonical geometric relationships such as local coplanarity or orthogonality is relevant for registration of heterogeneous or redundant data, as well as for improving the robustness of the reconstruction process.

3.3. Approximation

Our objective is to explore the approximation of complex shapes and scenes with surface and volume meshes, as well as on surface and domain tiling. A general way to state the shape approximation problem is to say that we search for the shape discretization (possibly with several levels of detail) that realizes the best complexity / distortion trade-off. Such a problem statement requires defining a discretization model, an error metric to measure distortion as well as a way to measure complexity. The latter is most commonly expressed in number of polygon primitives, but other measures closer to information theory lead to measurements such as number of bits or minimum description length.

For surface meshes we intend to conceive methods which provide control and guarantees both over the global approximation error and over the validity of the embedding. In addition, we seek for resilience to heterogeneous data, and robustness to noise and outliers. This would allow repairing and simplifying triangle soups with cracks, self-intersections and gaps. Another exploratory objective is to deal generically with different error metrics such as the symmetric Hausdorff distance, or a Sobolev norm which mixes errors in geometry and normals.

For surface and domain tiling the term meshing is substituted for tiling to stress the fact that tiles may be not just simple elements, but can model complex smooth shapes such as bilinear quadrangles. Quadrangle surface tiling is central for the so-called *resurfacing* problem in reverse engineering: the goal is to tile an input raw surface geometry such that the union of the tiles approximates the input well and such that each tile matches certain properties related to its shape or its size. In addition, we may require parameterization domains with a simple structure. Our goal is to devise surface tiling algorithms that are both reliable and resilient to defect-laden inputs, effective from the shape approximation point of view, and with flexible control upon the structure of the tiling.

3.4. Reconstruction

Assuming a geometric dataset made out of points or slices, the process of shape reconstruction amounts to recovering a surface or a solid that matches these samples. This problem is inherently ill-posed as infinitely-many shapes may fit the data. One must thus regularize the problem and add priors such as simplicity or smoothness of the inferred shape.

The concept of geometric simplicity has led to a number of interpolating techniques commonly based upon the Delaunay triangulation. The concept of smoothness has led to a number of approximating techniques that commonly compute an implicit function such that one of its isosurfaces approximates the inferred surface. Reconstruction algorithms can also use an explicit set of prior shapes for inference by assuming that the observed data can be described by these predefined prior shapes. One key lesson learned in the shape problem is that there is probably not a single solution which can solve all cases, each of them coming with its own distinctive features. In addition, some data sets such as point sets acquired on urban scenes are very domain-specific and require a dedicated line of research.

In recent years the *smooth, closed case* (i.e., shapes without sharp features nor boundaries) has received considerable attention. However, the state-of-the-art methods have several shortcomings: in addition to being in general not robust to outliers and not sufficiently robust to noise, they often require additional attributes as input, such as lines of sight or oriented normals. We wish to devise shape reconstruction methods which are both geometrically and topologically accurate without requiring additional attributes, while exhibiting resilience to defect-laden inputs. Resilience formally translates into stability with respect to noise and outliers. Correctness of the reconstruction translates into convergence in geometry and (stable parts of) topology of the reconstruction with respect to the inferred shape known through measurements.

Moving from the smooth, closed case to the *piecewise smooth case* (possibly with boundaries) is considerably harder as the ill-posedness of the problem applies to each sub-feature of the inferred shape. Further, very few approaches tackle the combined issue of robustness (to sampling defects, noise and outliers) and feature reconstruction.

TYREX Project-Team

3. Research Program

3.1. Modeling

Modeling consists in capturing various aspects of document and data processing and communication in a unifying model. Our modeling research direction mainly focuses on three aspects.

The first aspect aims at reducing the impedance mismatch. The impedance mismatch refers to the complexity, difficulty and lack of performance induced by various web application layers which require the same piece of information to be represented and processed differently. The mismatch occurs because programming languages use different native data models than those used for documents in browsers and for storage in databases. This results in complex and multi-tier software architectures whose different layers are incompatible in nature. This, in turn, results in expensive, inefficient, and error-prone web development. For reducing the impedance mismatch, we will focus on the design of a unifying software stack and programming framework, backed by generic and solid logical foundations similar in spirit to the NoSQL approach.

The second aspect aims at harnessing heterogeneity. Web applications increasingly use diverse data models: ordered and unordered tree-like structures (such as XML), nested records and arrays (such as JSON), graphs (like RDF), and tables. Furthermore, these data models involve a variety of languages for expressing constraints over data (e.g. XML schema, RelaxNG, and RDFS to name just a few). We believe that this heterogeneity is here to stay and is likely to increase. These differences in representations imply loads of error-prone and costly conversions and transformations. Furthermore, some native formats (e.g. JSON) are repurposed from an internal representation to a format for data exchange. This often results in a loss of information and in errors that need to be tracked and corrected. In this context, it is important to seek methods for reducing risks of information loss during data transformation and exchange. For harnessing heterogeneity, we will focus on the integration of data models through unified formal semantics and in particular logical interpretation. This allows using the same programming language constructs on different data models. At the programming language level, this is similar to languages such as JSonIq for JSON and XML.

Finally, the third aspect aims at making applications and data more compositional. Most web programming technologies are currently limited from a compositional point of view. For example, tree grammars (like schema languages for XML) are monolithic in the sense that they require the full description of the considered structures, instead of allowing the assembly of smaller and reusable building blocks. As a consequence, this translates into monolithic web applications, which makes their automated verification harder by making modular analyses more difficult. The need for compositionality is illustrated in the industry by the increasing development of fragmented W3C specifications organised in ad-hoc modules. For making applications and data more compositional, we will focus on the design of modular schema and programming languages. For this purpose, we will notably rely on succinct yet expressive formalisms (like two-way logics, polymorphic types, session types) that ease the process of expressing modular specifications.

3.2. Analysis, verification and optimization

This research direction aims at guaranteeing two different kinds of properties: safety and efficiency.

The first kind of properties concerns the safety of web applications. Software development was traditionally split between critical and non-critical software. Advanced (and costly) formal verification techniques were reserved to the former whereas non-critical software relied almost exclusively on testing, which only offers a ‘best-effort’ guarantee (removes most bugs but some of them may not be detected). The central idea was that in a non-critical system, the damage a failure may create is not worth the cost of formal verification. However, as web applications grow more pervasive in everyday life and gain momentum in corporates and various social organizations, and touch larger numbers of users, the potential cost of failure is rapidly and significantly increasing. In that sense, we can consider that web applications are becoming more and more critical. The growing dependency on the web as a tool, combined with the fact that some applications involve very large user bases, is becoming problematic as it seems to increase rapidly but silently. Some errors like crashes and confidential information leaks, if not discovered, can have massive effects and cause significant financial or reputation damage.

The second kind of properties concerns the efficiency of web applications. One particular characteristic of web programming languages is that they are essentially data-manipulation oriented. These manipulations rely on query and transformation languages whose performance is critical. This performance is very sensitive to data size and organization (constraints) and to the execution model (e.g. streaming evaluators). Static analysis can be used to optimize runtime performance by compile-time automated modification of the code (e.g. substitution of queries by more efficient ones). One major scientific difficulty here consists in dealing with problems close to the frontier of decidability, and therefore in finding useful trade-offs between programming ease, expressivity, complexity, succinctness, algorithmic techniques and effective implementations.

3.3. Design of advanced (robust, flexible, rich, novel) web applications

The generalized use of mobile terminals deeply affects the way users perceive and interact with their environment. The ubiquitous use of search engines capable of producing results in fractions of a second raised user expectations to a very high level: users now expect relevant information to be made available to them instantly and directly by context sensitivity to the environment itself. However, the information that needs to be processed is becoming more and more complex compared to the traditional web. In order to unlock the potential introduced by this new generation of the web, a radical rethinking of how web information is produced, organized and processed is necessary.

Until now, content rendering on the web was mainly based on supporting media formats separately. It is still notably the case in HTML5 for example where, for instance, vector graphics, mathematical content, audio and video are supported only as isolated media types. With the increasing use of web content in mobile terminals, we also need to take into account highly dynamic information flowing from sensors (positioning and orientation moves) and cameras. To reach that goal, web development platforms need to ease the manipulation of such content with carefully designed programming interfaces and by developing supporting integrative methods.

More precisely, we will focus on the following aspects: (1) **Build Rich content models**. This requires combining in a single model several content facets such as 3D elements, animations, user interactions, etc. We will focus on feature-compositional methods, which have become a prerequisite for the production of compelling web applications. (2) **Physical environment modeling and integration**. This consists of modeling and representing urban data such as buildings, pathways, points of interest. It requires developing appropriate languages and techniques to represent, process and query such environment models. In particular, we will focus on tracking positional user information and design techniques capable of combining semantic annotations, content, and representation of the physical world. (3) **Native streams support**. This consists of capturing new data flows extracted from various sensors in mobile terminals and various equipments. (4) **Cross-platform abstractions**. We will contribute to the design of appropriate abstractions to make applications run in a uniform way across various devices and environments. Our goal is to provide a viable alternative to current (platform-specific) mobile application development practices.

WILLOW Project-Team

3. Research Program

3.1. 3D object and scene modeling, analysis, and retrieval

This part of our research focuses on geometric models of specific 3D objects at the local (differential) and global levels, physical and statistical models of materials and illumination patterns, and modeling and retrieval of objects and scenes in large image collections. Our past work in these areas includes research aimed at recognizing rigid 3D objects in cluttered photographs taken from arbitrary viewpoints (Rothganger *et al.*, 2006), segmenting video sequences into parts corresponding to rigid scene components before recognizing these in new video clips (Rothganger *et al.*, 2007), retrieval of particular objects and buildings from images and videos (Sivic and Zisserman, 2003) and (Philbin *et al.*, 2007), and a theoretical study of a general formalism for modeling central and non-central cameras using the formalism and terminology of classical projective geometry (Ponce, 2009 and Batog *et al.*, 2010).

We have also developed multi-view stereopsis algorithms that have proven remarkably effective at recovering intricate details and thin features of compact objects and capturing the overall structure of large-scale, cluttered scenes. We have obtained a US patent 8,331,615 [0] for the corresponding software (PMVS, https://github.com/pmoulon/CMVS-PMVS) which is available under a GPL license and used for film production by ILM and Weta as well as by Google in Google Maps. It is also the basic technology used by Iconem, a start-up founded by Y. Ubelmann, a Willow collaborator. We have also applied our multi-view-stereo approach to model archaeological sites together with developing representations and efficient retrieval techniques to enable matching historical paintings to 3D models of archaeological sites (Russel *et al.*, 2011).

Our current efforts in this area are outlined in detail in Section. 7.1 .

3.2. Category-level object and scene recognition

The objective in this core part of our research is to learn and recognize quickly and accurately thousands of visual categories, including materials, objects, scenes, and broad classes of temporal events, such as patterns of human activities in picnics, conversations, etc. The current paradigm in the vision community is to model/learn one object category (read 2D aspect) at a time. If we are to achieve our goal, we have to break away from this paradigm, and develop models that account for the tremendous variability in object and scene appearance due to texture, material, viewpoint, and illumination changes within each object category, as well as the complex and evolving relationships between scene elements during the course of normal human activities.

Our current work in this area is outlined in detail in Section 7.2 .

3.3. Image restoration, manipulation and enhancement

The goal of this part of our research is to develop models, and methods for image/video restoration, manipulation and enhancement. The ability to “intelligently" manipulate the content of images and video is just as essential as high-level content interpretation in many applications: This ranges from restoring old films or removing unwanted wires and rigs from new ones in post production, to cleaning up a shot of your daughter at her birthday party, which is lovely but noisy and blurry because the lights were out when she blew the candles, or editing out a tourist from your Roman holiday video. Going beyond the modest abilities of current “digital zoom" (bicubic interpolation in general) so you can close in on that birthday cake, “deblock" a football game on TV, or turn your favorite DVD into a blue-ray, is just as important.

[0] The patent: "Match, Expand, and Filter Technique for Multi-View Stereopsis" was issued December 11, 2012 and assigned patent number 8,331,615.

In this context, we believe there is a new convergence between computer vision, machine learning, and signal processing. For example: The idea of exploiting self-similarities in image analysis, originally introduced in computer vision for texture synthesis applications (Efros and Leung, 1999), is the basis for non-local means (Buades *et al.*, 2005), one of today's most successful approaches to image restoration. In turn, by combining a powerful sparse coding approach to non-local means (Dabov *et al.*, 2007) with modern machine learning techniques for dictionary learning (Mairal *et al.*, 2010), we have obtained denoising and demosaicking results that are the state of the art on standard benchmarks (Mairal *et al.*, 2009).

Our current work is outlined in detail in Section 7.3 .

3.4. Human activity capture and classification

From a scientific point of view, visual action understanding is a computer vision problem that until recently has received little attention outside of extremely specific contexts such as surveillance or sports. Many of the current approaches to the visual interpretation of human activities are designed for a limited range of operating conditions, such as static cameras, fixed scenes, or restricted actions. The objective of this part of our project is to attack the much more challenging problem of understanding actions and interactions in unconstrained video depicting everyday human activities such as in sitcoms, feature films, or news segments. The recent emergence of automated annotation tools for this type of video data (Everingham, Sivic, Zisserman, 2006; Laptev, Marszałek, Schmid, Rozenfeld, 2008; Duchenne, Laptev, Sivic, Bach, Ponce, 2009) means that massive amounts of labelled data for training and recognizing action models will at long last be available.

Our research agenda in this scientific domain is described below and our recent results are outlined in detail in Section 7.4 .

- **Weakly-supervised learning and annotation of human actions in video.** We aim to leverage the huge amount of video data using readily-available annotations in the form of video scripts. Scripts, however, often provide only imprecise and incomplete information about the video. We address this problem with weakly-supervised learning techniques both at the text and image levels.
- **Descriptors for video representation** Video representation has a crucial role for recognizing human actions and other components of a visual scene. Our work in this domain aims to develop generic methods for representing video data based on realistic assumptions. In particular, we develop deep learning methods and design new trainable representations for various tasks such as human action recognition, person detection, segmentation and tracking.

WIMMICS Project-Team

3. Research Program

3.1. Users Modeling and Designing Interaction on the Web

Wimmics focuses on interactions of ordinary users with ontology-based knowledge systems with a preference for semantic Web formalisms and Web 2.0 applications. We specialize interaction design and evaluation methods to Web application tasks such as searching, browsing, contributing or protecting data. The team is especially interested in using semantics in assisting the interactions. We propose knowledge graph representations and algorithms to support interaction adaptation for instance for context-awareness or intelligent interactions with machine. We propose and evaluate Web-based visualization techniques for linked data, querying, reasoning, explaining and justifying. Wimmics also integrates natural language processing approaches to support natural language based interactions. We rely on cognitive studies to build models of the system, the user and the interactions between users through the system, in order to support and improve these interactions. We extend the user modeling technique known as *Personas* where user models are represented as specific, individual humans. *Personas* are derived from significant behavior patterns (i.e., sets of behavioral variables) elicited from interviews with and observations of users (and sometimes customers) of the future product. Our user models specialize *Personas* approaches to include aspects appropriate to Web applications. Wimmics also extends user models to capture very different aspects (e.g. emotional states).

3.2. Communities and Social Interactions Analysis

The domain of social network analysis is a whole research domain in itself and Wimmics targets what can be done with typed graphs, knowledge representations and social models. We also focus on the specificity of social Web and semantic Web applications and in bridging and combining the different social Web data structures and semantic Web formalisms. Beyond the individual user models, we rely on social studies to build models of the communities, their vocabularies, activities and protocols in order to identify where and when formal semantics is useful. We propose models of collectives of users and of their collaborative functioning extending the collaboration personas and methods to assess the quality of coordination interactions and the quality of coordination artifacts. We extend and compare community detection algorithms to identify and label communities of interest with the topics they share. We propose mixed representations containing social semantic representations (e.g. folksonomies) and formal semantic representations (e.g. ontologies) and propose operations that allow us to couple them and exchange knowledge between them. Moving to social interaction we develop models and algorithms to mine and integrate different yet linked aspects of social media contributions (opinions, arguments and emotions) relying in particular on natural language processing and argumentation theory. To complement the study of communities we rely on multi-agent systems to simulate and study social behaviors. Finally we also rely on Web 2.0 principles to provide and evaluate social Web applications.

3.3. Vocabularies, Semantic Web and Linked Data Based Knowledge Representation

For all the models we identified in the previous sections, we rely on and evaluate knowledge representation methodologies and theories, in particular ontology-based modeling. We also propose models and formalisms to capture and merge representations of different levels of semantics (e.g. formal ontologies and social folksonomies). The important point is to allow us to capture those structures precisely and flexibly and yet create as many links as possible between these different objects. We propose vocabularies and semantic Web formalizations for the whole aspects we model and we consider and study extensions of these formalisms when needed. The results have all in common to pursue the representation and publication of our models as linked data. We also contribute to the transformation and linking of existing resources (informal models, databases, texts, etc.) to be published on the semantic Web and as linked data. Examples of aspects we formalize include: user profiles, social relations, linguistic knowledge, business processes, derivation rules, temporal descriptions, explanations, presentation conditions, access rights, uncertainty, emotional states, licenses, learning resources, etc. At a more conceptual level we also work on modeling the Web architecture with philosophical tools so as to give a realistic account of identity and reference and to better understand the whole context of our research and its conceptual cornerstones.

3.4. Analyzing and Reasoning on Heterogeneous Semantic Graphs

One of the characteristics of Wimmics is to rely on graph formalisms unified in an abstract graph model and operators unified in an abstract graph machine to formalize and process semantic Web data, Web resources, services metadata and social Web data. In particular Corese, the core software of Wimmics, maintains and implements that abstraction. We propose algorithms to process the mixed representations of the previous section. In particular we are interested in allowing cross-enrichment between them and in exploiting the life cycle and specificity of each one to foster the life-cycles of the others. Our results all have in common to pursue analyzing and reasoning on heterogeneous semantic graphs issued from social and semantic Web applications. Many approaches emphasize the logical aspect of the problem especially because logics are close to computer languages. We defend that the graph nature of Linked Data on the Web and the large variety of types of links that compose them call for typed graphs models. We believe the relational dimension is of paramount importance in these representations and we propose to consider all these representations as fragments of a typed graph formalism directly built above the Semantic Web formalisms. Our choice of a graph based programming approach for the semantic and social Web and of a focus on one graph based formalism is also an efficient way to support interoperability, genericity, uniformity and reuse.

ZENITH Project-Team

3. Research Program

3.1. Data Management

Data management is concerned with the storage, organization, retrieval and manipulation of data of all kinds, from small and simple to very large and complex. It has become a major domain of computer science, with a large international research community and a strong industry. Continuous technology transfer from research to industry has led to the development of powerful DBMS, now at the heart of any information system, and of advanced data management capabilities in many kinds of software products (search engines, application servers, document systems, etc.).

The fundamental principle behind data management is *data independence*, which enables applications and users to deal with the data at a high conceptual level while ignoring implementation details. The relational model, by resting on a strong theory (set theory and first-order logic) to provide data independence, has revolutionized data management. The major innovation of relational DBMS has been to allow data manipulation through queries expressed in a high-level (declarative) language such as SQL. Queries can then be automatically translated into optimized query plans that take advantage of underlying access methods and indices. Many other advanced capabilities have been made possible by data independence : data and metadata modeling, schema management, consistency through integrity rules and triggers, transaction support, etc.

This data independence principle has also enabled DBMS to continuously integrate new advanced capabilities such as object and XML support and to adapt to all kinds of hardware/software platforms from very small smart devices (smart phone, PDA, smart card, etc.) to very large computers (multiprocessor, cluster, etc.) in distributed environments. For a long time, the research focus was on providing advanced database capabilities with good performance, for both transaction processing and decision support applications. And the main objective was to support all these capabilities within a single DBMS.

The problems of scientific data management (massive scale, complexity and heterogeneity) go well beyond the traditional context of DBMS. To address them, we capitalize on scientific foundations in closely related domains: distributed data management, cloud data management, big data, big data integration, scientific workflows, data analytics and search.

3.2. Distributed Data Management

To deal with the massive scale of scientific data, we exploit large-scale distributed systems, with the objective of making distribution transparent to the users and applications. Thus, we capitalize on the principles of large-scale distributed systems such as clusters, peer-to-peer (P2P) and cloud.

Data management in distributed systems has been traditionally achieved by distributed database systems which enable users to transparently access and update several databases in a network using a high-level query language (e.g. SQL) [12]. Transparency is achieved through a global schema which hides the local databases' heterogeneity. In its simplest form, a distributed database system is a centralized server that supports a global schema and implements distributed database techniques (query processing, transaction management, consistency management, etc.). This approach has proved to be effective for applications that can benefit from centralized control and full-fledge database capabilities, e.g. information systems. However, it cannot scale up to more than tens of databases.

Parallel database systems extend the distributed database approach to improve performance (transaction throughput or query response time) by exploiting database partitioning using a multiprocessor or cluster system. Although data integration systems and parallel database systems can scale up to hundreds of data sources or database partitions, they still rely on a centralized global schema and strong assumptions about the network.

In contrast, peer-to-peer (P2P) systems [8] adopt a completely decentralized approach to data sharing. By distributing data storage and processing across autonomous peers in the network, they can scale without the need for powerful servers. Popular examples of P2P systems such as Gnutella and BitTorrent have millions of users sharing petabytes of data over the Internet. Although very useful, these systems are quite simple (e.g. file sharing), support limited functions (e.g. keyword search) and use simple techniques (e.g. resource location by flooding) which have performance problems. A P2P solution is well-suited to support the collaborative nature of scientific applications as it provides scalability, dynamicity, autonomy and decentralized control. Peers can be the participants or organizations involved in collaboration and may share data and applications while keeping full control over their (local) data sources. But for very-large scale scientific data analysis, we believe cloud computing (see next section), is the right approach as it can provide virtually infinite computing, storage and networking resources. However, current cloud architectures are proprietary, ad-hoc, and may deprive users of the control of their own data. Thus, we postulate that a hybrid P2P/cloud architecture is more appropriate for scientific data management, by combining the best of both approaches. In particular, it will enable the clean integration of the users' own computational resources with different clouds.

3.3. Cloud Data Management

Cloud computing encompasses on demand, reliable services provided over the Internet (typically represented as a cloud) with easy access to virtually infinite computing, storage and networking resources. Through very simple Web interfaces and at small incremental cost, users can outsource complex tasks, such as data storage, system administration, or application deployment, to very large data centers operated by cloud providers. However, cloud computing has some drawbacks and not all applications are good candidates for being "cloudified". The major concern is w.r.t. data security and privacy, and trust in the provider (which may use no so trustful providers to operate). One earlier criticism of cloud computing was that customers get locked in proprietary clouds. It is true that most clouds are proprietary and there are no standards for cloud interoperability.

There is much more variety in cloud data than in scientific data since there are many different kinds of customers (individuals, samll companies, large corporations, etc.). However, we can identify common features. Cloud data can be very large, unstructured (e.g. text-based) or semi-structured, and typically append-only (with rare updates). And cloud users and application developers may be in high numbers, but not DBMS experts.

3.4. Big Data

Big data (like its relative, data science) has become a buzz word, with different meanings depending on your perspective, e.g. 100 terabytes is big for a transaction processing system, but small for a web search engine. It is also a moving target, as shown by two landmarks in DBMS products: the Teradata database machine in the 1980's and the Oracle Exadata database machine in 2010.

Although big data has been around for a long time, it is now more important than ever. We can see overwhelming amounts of data generated by all kinds of devices, networks and programs, e.g. sensors, mobile devices, connected objects (IoT), social networks, computer simulations, satellites, radiotelescopes, etc. Storage capacity has doubled every 3 years since 1980 with prices steadily going down (e.g. 1 Gigabyte of Hard Disk Drive for: 1M$ in 1982, 1K$ in 1995, 0.02$ in 2015), making it affordable to keep more data around. And massive data can produce high-value information and knowledge, which is critical for data analysis, decision support, forecasting, business intelligence, research, (data-intensive) science, etc.

The problem of big data has three main dimensions, quoted as the three big V's:

- Volume: refers to massive amounts of data, making it hard to store, manage, and analyze (big analytics);
- Velocity: refers to continuous data streams being produced, making it hard to perform online processing and analysis;
- Variety: refers to different data formats, different semantics, uncertain data, multiscale data, etc., making it hard to integrate and analyze.

There are also other V's such as: validity (is the data correct and accurate?); veracity (are the results meaningful?); volatility (how long do you need to store this data?).

Many different big data management solutions have been designed, primarily for the cloud, as cloud and big data are synergistic. They typically trade consistency for scalability, simplicity and flexibility, hence the new term Data-Intensive Scalable Computing (DISC). Examples of DISC systems include data processing frameworks (e.g. Hadoop MapReduce, Apache Spark, Pregel), file systems (e.g. Google GFS, HDFS), NoSQL systems (Google BigTable, Hbase, MongoDB), NewSQL systems (Google F1, CockroachDB, LeanXcale). In Zenith, we exploit or extend DISC technologies to fit our needs for scientific workflow management and scalable data analysis.

3.5. Data Integration

Scientists can rely on web tools to quickly share their data and/or knowledge. Therefore, when performing a given study, a scientist would typically need to access and integrate data from many data sources (including public databases). Data integration can be either physical or logical. In the former, the source data are integrated and materialized in a data warehouse. In logical integration, the integrated data are not materialized, but accessed indirectly through a global (or mediated) schema using a data integration system. These two approaches have different trade-offs, e.g. efficient analytics but only on historical data for data warehousing versus real-time access to data sources for data integration systems (e.g. web price comparators).

In both cases, to understand a data source content, metadata (data that describe the data) is crucial. Metadata can be initially provided by the data publisher to describe the data structure (e.g. schema), data semantics based on ontologies (that provide a formal representation of the domain knowledge) and other useful information about data provenance (publisher, tools, methods, etc.). Scientific metadata is very heterogeneous, in particular because of the autonomy of the underlying data sources, which leads to a large variety of models and formats. Thus, it is necessary to identify semantic correspondences between the metadata of the related data sources. This requires the matching of the heterogeneous metadata, by discovering semantic correspondences between ontologies, and the annotation of data sources using ontologies. In Zenith, we rely on semantic web techniques (e.g. RDF and SparkQL) to perform these tasks and deal with high numbers of data sources.

Scientific workflow management systems (SWfMS) are also useful for data integration. They allow scientists to describe and execute complex scientific activities, by automating data derivation processes, and supporting various functions such as provenance management, queries, reuse, etc. Some workflow activities may access or produce huge amounts of distributed data. This requires using distributed and parallel execution environments. However, existing workflow management systems have limited support for data parallelism. In Zenith, we use an algebraic approach to describe data-intensive workflows and exploit parallelism.

3.6. Data Analytics

Data analytics refers to a set of techniques to draw conclusions through data examination. It involves data mining, statistics, and data management. Data mining provides methods to discover new and useful patterns from very large datasets. These patterns may take different forms, depending on the end-user's request, such as:

- **Frequent itemsets and association rules**. In this case, the data is usually a table with a high number of rows and the data mining algorithm extracts correlations between column values. This problem was first motivated by commercial and marketing purposes (*e.g.* discovering frequent correlations between items bought in a shop, which could help selling more). A typical example of frequent itemset from a sensor network in a smart building would say that "in 20% rooms, the door is closed, the room is empty, and lights are on."
- **Frequent sequential pattern extraction.** This problem is very similar to frequent itemset discovery but considering the order between. In the smart building example, a frequent sequence could say that "in 40% of rooms, lights are on at time i, the room is empty at time i+j and the door is closed at time i+j+k". Discovering frequent sequences has become critical in marketing, as well as in security (e.g.

detecting network intrusions), in web usage analysis and any domain where data come in a specific order, typically given by timestamps.

- **Clustering**. The goal of clustering is to group together similar data while ensuring that dissimilar data will not be in the same cluster. In our example of smart buildings, we could find clusters of rooms, where offices will be in one category and copy machine rooms in another because of their differences (hours of people presence, number of times lights are turned on/off, etc.).

One main problem in data analytics is to deal with data streams. Existing methods have been designed for very large data sets where complex algorithms from artificial intelligence were not efficient because of data size. However, we now must deal with data streams, sequences of data events arriving at high rate, where traditional data analytics techniques cannot complete in real-time, given the infinite data size. In order to extract knowledge from data streams, the data mining community has investigated approximation methods that could yield good result quality.

3.7. Data Search

Technologies for searching information in scientific data have relied on relational DBMS or text-based indexing methods. However, content-based information retrieval has progressed much in the last decade, with much impact on search engines. Rather than restricting the search to the use of metadata, content-based methods index, search and browse digital objects by means of signatures that describe their content. Such methods have been intensively studied in the multimedia community to allow searching massive amounts of multimedia documents that are created every day (e.g. 99% of web data are audio-visual content with very sparse metadata). Scalable content-based methods have been proposed for searching objects in large image collections or detecting copies in huge video archives. Besides multimedia contents, content-based information retrieval methods have expanded their scope to deal with more diverse data such as medical images, 3D models or even molecular data. Potential applications in scientific data management are numerous. First, to allow searching within huge collections of scientific images (earth observation, medical images, botanical images, biology images, etc.) or browsing large datasets of experimental data (e.g. multisensor data, molecular data or instrumental data). However, scalability remains a major issue, involving complex algorithms (such as similarity search, clustering or supervised retrieval), in high dimensional spaces (up to millions of dimensions) with complex metrics (Lp, Kernels, sets intersections, edit distances, etc.). Most of these algorithms have linear, quadratic or even cubic complexities so that their use at large scale is not affordable without major breakthroughs. In Zenith, we investigate the following challenges:

- **High-dimensional similarity search**. Whereas many indexing methods were designed in the last 20 years to efficiently retrieve multidimensional data with relatively small dimensions, high-dimensional data are challenged by the well-known curse of dimensionality . Only recently have some methods appeared that allow approximate Nearest Neighbors queries in sub-linear time, in particular, Locality Sensitive Hashing methods that offer new theoretical insights in high-dimensional Euclidean spaces and random projections. But there are still challenging issues such as efficient similarity search in any kernel or metric spaces, efficient construction of k-nearest neighbor graphs (k-NNG) or relational similarity queries.
- **Large-scale supervised retrieval**. Supervised retrieval aims at retrieving relevant objects in a dataset by providing some positive and/or negative training samples. Toward this goal, Support Vector Machines (SVM) offer the possibility to construct generalized, non-linear predictors in high-dimensional spaces using small training sets. The prediction time complexity of these methods is usually linear in dataset size. Allowing hyperplane similarity queries in sub-linear time is for example a challenging research issue. A symmetric problem in supervised retrieval consists in retrieving the most relevant object categories that might contain a given query object, providing huge labeled datasets (up to millions of classes and billions of objects) and very few objects per category (from 1 to 100 objects). SVM methods that are formulated as quadratic programming with cubic training time complexity and quadratic space complexity are clearly not usable. Promising solutions include hybrid supervised-unsupervised methods and supervised hashing methods.

- **Distributed content-based retrieval**. Distributed content-based retrieval methods appear as a promising solution to manage masses of data distributed over large networks, in particular when the data cannot be centralized for privacy or cost reasons, which is often the case in scientific social networks. However, current methods are limited to very simple similarity search paradigms. In Zenith, we consider more advanced distributed content-based retrieval and mining methods such as k-NNG construction, large-scale supervised retrieval or multi-source clustering.