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FIELD

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Section Scientific Foundations

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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)

Implementing "ultimately accurate" functions (i.e., rounded to nearest) requires either the knowledge of hardest-to-round cases, or an as tight as possible lower bound on the distance between the image of a floating-point number by the function and the middle of two consecutive floating-point numbers. Obtaining such results is a challenge. Several computer manufacturers have contacted us to obtain new cases. One of our current solutions for obtaining hardest-to-round cases is based on Lefèvre's algorithm. We aim at rewriting the current implementations of this algorithm, and giving formal proofs of their correction.

We plan to use uniform polynomial approximation and diophantine techniques in order to tackle the case of the IEEE quad precision, and continue to use 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.
- 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

We aim at providing tight error bounds for basic “buiding blocks” of numerical computing. Examples are complex arithmetic (in the continuity of what we have already done), Fourier transforms.

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.

CASH Team

3. Research Program

3.1. Definition of dataflow representations of parallel programs

In the last decades, several frameworks have emerged to design efficient compiler algorithms. The efficiency of all the optimizations performed in compilers strongly relies on effective *static analyses* and *intermediate representations*. Dataflow models are a natural intermediate representation for hardware compilers (HLS) and more generally for parallelizing compilers. Indeed, dataflow models capture task-level parallelism and can be mapped naturally to parallel architectures. In a way, a dataflow model is a partition of the computation into processes and a partition of the flow dependences into channels. This partitioning prepares resource allocation (which processor/hardware to use) and medium-grain communications.

The main goal of the CASH team is to provide efficient analyses and the optimizing compilation frameworks for dataflow programming models. The results of the team will rely on programming languages and representation of programs in which parallelism and dataflow play a crucial role. This first research direction aims at defining these dataflow languages and intermediate representations, both from a practical perspective (syntax or structure), and from a theoretical point of view (semantics). This first research direction thus defines the models on which the other directions will rely. It is important to note that we do not restrict ourself to a strict definition of dataflow languages and, more generally, we are interested in the parallel languages in which dataflow synchronization plays a significant role.

Intermediate dataflow model. The intermediate dataflow model is a representation of the program that is adapted for optimization and scheduling. It will be obtained from the analysis of a (parallel or sequential) program and should at some point be used for compilation. The dataflow model must specify precisely its semantics and parallelism granularity. It must also be analyzable with polyhedral techniques, where powerful concepts exist to design compiler analysis, e.g., scheduling or resource allocation. Polyhedral Process Networks [55] extended with a module system could be a good starting point. But then, how to fit non-polyhedral parts of the program? A solution is to hide non-polyhedral parts into processes with a proper polyhedral abstraction. This organization between polyhedral and non-polyhedral processes will be a key aspect of our medium-grain dataflow model. The design of our intermediate dataflow model and the precise definition of its semantics will constitute a reliable basis to formally define and ensure the correctness of algorithms proposed by CASH: compilation, optimizations and analyses.

Dataflow programming languages. Dataflow paradigm has also been explored quite intensively in programming languages. Indeed, there exists a large panel of dataflow languages, whose characteristics differ notably, the major point of variability being the scheduling of agents and their communications. There is indeed a continuum from the synchronous dataflow languages like Lustre [37] or Streamit [51], where the scheduling is fully static, and general communicating networks like KPNs [39] or RVC-Cal [19] where a dedicated runtime is responsible for scheduling tasks dynamically, when they *can* be executed. These languages share some similarities with actor languages that go even further in the decoupling of processes by considering them as independent reactive entities. Another objective of the CASH team is to study dataflow programming *languages*, their semantics, their expressiveness, and their compilation. The specificity of the CASH team will be that these languages will be designed taking into consideration the compilation using polyhedral techniques. In particular, we will explore which dataflow constructs are better adapted for our static analysis, compilation, and scheduling techniques. In practice we want to propose high-level primitives to express data dependency, this way the programmer will express parallelism in a dataflow way instead of the classical communication-oriented dependencies. The higher-level more declarative point of view will make programming easier but also give more optimization opportunities. These primitives will be inspired by the existing works in the polyhedral model framework, as well as dataflow languages, but also in the actors and active object languages [26] that nowadays introduce more and more dataflow primitives to enable data-driven interactions between agents, particularly with *futures* [24], [31].

3.1.1. Expected Impact

Consequently, the impact of this research direction is both the usability of our representation for static analyses and optimizations performed in Sections 3.2 and 3.3 , and the usability of its semantics to prove the correctness of these analyses.

3.1.2. Scientific Program

3.1.2.1. Short-term and ongoing activities.

We obtained preliminary experimental [16], [17], [32] and theoretical [38] results, exploring several aspects of dataflow models. The next step is to define accurately the intermediate dataflow model and to study existing programming and execution models:

- Define our medium-grain dataflow model. So far, a modular Polyhedral Process Networks appears as a natural candidate but it may need to be extended to be adapted to a wider range of applications. Precise semantics will have to be defined for this model to ensure the articulation with the activities discussed in Section 3.3 .
- Study precisely existing dataflow languages, their semantics, their programmability, and their limitations.

3.1.2.2. Medium-term activities.

In a second step, we will extend the existing results to widen the expressiveness of our intermediate representation and design new parallelism constructs. We will also work on the semantics of dataflow languages:

- Propose new stream programming models and a clean semantics where all kinds of parallelisms are expressed explicitly, and where all activities from code design to compilation and scheduling can be clearly expressed.
- Identify a core language that is rich enough to be representative of the dataflow languages we are interested in, but abstract and small enough to enable formal reasoning and proofs of correctness for our analyses and optimizations.

3.1.2.3. Long-term activities.

In a longer-term vision, the work on semantics, while remaining driven by the applications, would lead to to more mature results, for instance:

- Design more expressive dataflow languages and intermediate representations which would at the same time be expressive enough to capture all the features we want for aggressive HPC optimizations, and sufficiently restrictive to be (at least partially) statically analyzable at a reasonable cost.
- Define a module system for our medium-grain dataflow language. A program will then be divided into modules that can follow different compilation schemes and execution models but still communicate together. This will allow us to encapsulate a program that does not fit the polyhedral model into a polyhedral one and vice versa. Also, this will allow a compositional analysis and compilation, as opposed to global analysis which is limited in scalability.

3.2. Expressivity and Scalability of Static Analyses

The design and implementation of efficient compilers becomes more difficult each day, as they need to bridge the gap between *complex languages* and *complex architectures*. Application developers use languages that bring them close to the problem that they need to solve which explains the importance of high-level programming languages. However, high-level programming languages tend to become more distant from the hardware which they are meant to command.

In this research direction, we propose to design expressive and scalable static analyses for compilers. This topic is closely linked to Sections 3.1 and 3.3 since the design of an efficient intermediate representation is made while regarding the analyses it enables. The intermediate representation should be expressive enough to embed maximal information; however if the representation is too complex the design of scalable analyses will be harder.

The analyses we plan to design in this activity will of course be mainly driven by the HPC dataflow optimizations we mentioned in the preceding sections; however we will also target other kinds of analyses applicable to more general purpose programs. We will thus consider two main directions:

- Extend the applicability of the polyhedral model, in order to deal with HPC applications that do not fit totally in this category. More specifically, we plan to work on more complex control and also on complex data structures, like sparse matrices, which are heavily used in HPC.
- Design of specialized static analyses for memory diagnostic and optimization inside general purpose compilers.

For both activities, we plan to cross fertilize ideas coming from the abstract interpretation community as well as language design, dataflow semantics, and WCET estimation techniques.

Correct by construction analyses. The design of well-defined semantics for the chosen programming language and intermediate representation will allow us to show the correctness of our analyses. The precise study of the semantics of Section 3.1 will allow us to adapt the analysis to the characteristics of the language, and prove that such an adaptation is well founded. This approach will be applicable both on the source language and on the intermediate representation.

Such wellfoundedness criteria relatively to the language semantics will first be used to design our analyses, and then to study which extensions of the languages can be envisioned and analyzed safely, and which extensions (if any) are difficult to analyze and should be avoided. Here the correct identification of a core language for our formal studies (see Section 3.1) will play a crucial role as the core language should feature all the characteristics that might make the analysis difficult or incorrect.

Scalable abstract domains. We already have experience in designing low-cost semi relational abstract domains for pointers [44], [42], as well as tailoring static analyses for specialized applications in compilation [30], [50], Synchronous Dataflow scheduling [49], and extending the polyhedral model to irregular applications [15]. We also have experience in the design of various static verification techniques adapted to different programming paradigms.

3.2.1. Expected impact

The impact of this work is the significantly widened applicability of various tools/compilers related to parallelization: allow optimizations for a larger class of programs, and allow low-cost analysis that scale to very large programs.

We target both analysis for optimization and analysis to detect, or prove the absence of bugs.

3.2.2. Scientific Program

3.2.2.1. Short-term and ongoing activities.

Together with Paul Iannetta and Lionel Morel (INSA/CEA LETI), we are currently working on the *semantic rephrasing* of the polyhedral model [34]. The objective is to clearly redefine the key notions of the polyhedral model on general flowchart programs operating on arrays, lists and trees. We reformulate the algorithms that are performed to compute dependencies in a more semantic fashion, i.e. considering the program semantics instead of syntactical criteria. The next step is to express classical scheduling and code generation activities in this framework, in order to overcome the classical syntactic restrictions of the polyhedral model.

3.2.2.2. Medium-term activities.

In medium term, we want to extend the polyhedral model for more general data-structures like lists and sparse matrices. For that purpose, we need to find polyhedral (or other shapes) abstractions for non-array data-structures; the main difficulty is to deal with non-linearity and/or partial information (namely, over-approximations of the data layout, or over-approximation of the program behavior). This activity will rely on a formalization of the optimization activities (dependency computation, scheduling, compilation) in a more general Abstract-Interpretation based framework in order to make the approximations explicit.

At the same time, we plan to continue to work on scaling static analyses for general purpose programs, in the spirit of Maroua Maalej's PhD [41], whose contribution is a sequence of memory analyses inside production compilers. We already began a collaboration with Sylvain Collange (PACAP team of IRISA Laboratory) on the design of static analyses to optimize copies from the global memory of a GPU to the block kernels (to increase locality). In particular, we have the objective to design specialized analyses but with an explicit notion of cost/precision compromise, in the spirit of the paper [36] that tries to formalize the cost/precision compromise of interprocedural analyses with respect to a "context sensitivity parameter".

3.2.2.3. Long-term activities.

In a longer-term vision, the work on scalable static analyses, whether or not directed from the dataflow activities, will be pursued in the direction of large general-purpose programs.

An ambitious challenge is to find a generic way of adapting existing (relational) abstract domains within the Single Static Information [20] framework so as to improve their scalability. With this framework, we would be able to design static analyses, in the spirit of the seminal paper [25] which gave a theoretical scheme for classical abstract interpretation analyses.

We also plan to work on the interface between the analyses and their optimization clients inside production compilers.

3.3. Compiling and Scheduling Dataflow Programs

In this part, we propose to design the compiler analyses and optimizations for the *medium-grain* dataflow model defined in section 3.1 . We also propose to exploit these techniques to improve the compilation of dataflow languages based on actors. Hence our activity is split into the following parts:

- Translating a sequential program into a medium-grain dataflow model. The programmer cannot be expected to rewrite the legacy HPC code, which is usually relatively large. Hence, compiler techniques must be invented to do the translation.
- Transforming and scheduling our medium-grain dataflow model to meet some classic optimization criteria, such as throughput, local memory requirements, or I/O traffic.
- Combining agents and polyhedral kernels in dataflow languages. We propose to apply the techniques above to optimize the processes in actor-based dataflow languages and combine them with the parallelism existing in the languages.

We plan to rely extensively on the polyhedral model to define our compiler analysis. The polyhedral model was originally designed to analyze imperative programs. Analysis (such as scheduling or buffer allocation) must be redefined in light of dataflow semantics.

Translating a sequential program into a medium-grain dataflow model. The programs considered are compute-intensive parts from HPC applications, typically big HPC kernels of several hundreds of lines of C code. In particular, we expect to analyze the process code (actors) from the dataflow programs. On short ACL (Affine Control Loop) programs, direct solutions exist [53] and rely directly on array dataflow analysis [29]. On bigger ACL programs, this analysis no longer scales. We plan to address this issue by *modularizing* array dataflow analysis. Indeed, by splitting the program into processes, the complexity is mechanically reduced. This is a general observation, which was exploited in the past to compute schedules [28]. When the program is no longer ACL, a clear distinction must be made between polyhedral parts and non polyhedral parts. Hence, our medium-grain dataflow language must distinguish between polyhedral process networks, and non-polyhedral code fragments. This structure raises new challenges: How to abstract away non-polyhedral parts while keeping the polyhedrality of the dataflow program? Which trade-off(s) between precision and scalability are effective?

Medium-grain data transfers minimization. When the system consists of a single computing unit connected to a slow memory, the roofline model [56] defines the optimal ratio of computation per data transfer (*operational intensity*). The operational intensity is then translated to a partition of the computation (loop tiling) into *reuse units*: inside a reuse unit, data are transfered locally; between reuse units, data are transfered through the slow memory. On a *fine-grain* dataflow model, reuse units are exposed with loop tiling; this is the case for example

in Data-aware Process Network (DPN) [17]. The following questions are however still open: How does that translate on *medium-grain* dataflow models? And fundamentally what does it mean to *tile* a dataflow model?

Combining agents and polyhedral kernels in dataflow languages. In addition to the approach developed above, we propose to explore the compilation of dataflow programming languages. In fact, among the applications targeted by the project, some of them are already thought or specified as dataflow actors (video compression, machine-learning algorithms,...).

So far, parallelization techniques for such applications have focused on taking advantage of the decomposition into agents, potentially duplicating some agents to have several instances that work on different data items in parallel [35]. In the presence of big agents, the programmer is left with the splitting (or merging) of these agents by-hand if she wants to further parallelize her program (or at least give this opportunity to the runtime, which in general only sees agents as non-malleable entities). In the presence of arrays and loop-nests, or, more generally, some kind of regularity in the agent's code, however, we believe that the programmer would benefit from automatic parallelization techniques such as those proposed in the previous paragraphs. To achieve the goal of a totally integrated approach where programmers write the applications they have in mind (application flow in agents where the agents' code express potential parallelism), and then it is up to the system (compiler, runtime) to propose adequate optimizations, we propose to build on solid formal definition of the language semantics (thus the formal specification of parallelism occurring at the agent level) to provide hierarchical solutions to the problem of compilation and scheduling of such applications.

3.3.1. Expected impact

In general, splitting a program into simpler processes simplifies the problem. This observation leads to the following points:

- By abstracting away irregular parts in processes, we expect to structure the long-term problem of handling irregular applications in the polyhedral model. The long-term impact is to widen the applicability of the polyhedral model to irregular kernels.
- Splitting a program into processes reduces the problem size. Hence, it becomes possible to scale traditionally expensive polyhedral analysis such as scheduling or tiling to quote a few.

As for the third research direction, the short term impact is the possibility to combine efficiently classical dataflow programming with compiler polyhedral-based optimizations. We will first propose ad-hoc solutions coming from our HPC application expertise, but supported by strong theoretical results that prove their correctness and their applicability in practice. In the longer term, our work will allow specifying, designing, analyzing, and compiling HPC dataflow applications in a unified way. We target semi-automatic approaches where pertinent feedback is given to the developer during the development process.

3.3.2. Scientific Program

3.3.2.1. Short-term and ongoing activities.

We are currently working on the RTM (Reverse-Time Migration) kernel for oil and gas applications ($\approx$ 500 lines of C code). This kernel is long enough to be a good starting point, and small enough to be handled by a polyhedral splitting algorithm. We figured out the possible splittings so the polyhedral analysis can scale and irregular parts can be hidden. In a first step, we plan to define splitting metrics and algorithms to optimize the usual criteria: communication volume, latency and throughput.

Together with Lionel Morel (INSA/CEA LETI), we currently work on the evaluation of the practical advantage of combining the dataflow paradigm with the polyhedral optimization framework. We empirically build a proof-of-concept tooling approach, using existing tools on existing languages [33]. We combine dataflow programming with polyhedral compilation in order to enhance program parallelization by leveraging both inter-agent parallelism and intra-agent parallelism (i.e., regarding loop nests inside agents). We evaluate the approach practically, on benchmarks coming from image transformation or neural networks, and the first results demonstrate that there is indeed a room for further improvement.

3.3.2.2. Medium-term activities.

The results of the preceding paragraph are partial and have been obtained with a simple experimental approach only using off-the-shelf tools. We are thus encouraged to pursue research on combining expertise from dataflow programming languages and polyhedral compilation. Our long term objective is to go towards a formal framework to express, compile, and run dataflow applications with intrinsic instruction or pipeline parallelism.

We plan to investigate in the following directions:

- Investigate how polyhedral analysis extends on modular dataflow programs. For instance, how to modularize polyhedral scheduling analysis on our dataflow programs?
- Develop a proof of concept and validate it on linear algebra kernels (SVD, Gram-Schmidt, etc.).
- Explore various areas of applications from classical dataflow examples, like radio and video processing, to more recent applications in deep learning algorithmic. This will enable us to identify some potential (intra and extra) agent optimization patterns that could be leveraged into new language idioms.

3.3.2.3. Long-term activities.

Current work focus on purely polyhedral applications. Irregular parts are not handled. Also, a notion of tiling is required so the communications of the dataflow program with the outside world can be tuned with respect to the local memory size. Hence, we plan to investigate the following points:

- Assess simple polyhedral/non polyhedral partitioning: How non-polyhedral parts can be hidden in processes/channels? How to abstract the dataflow dependencies between processes? What would be the impact on analyses? We target programs with irregular control (e.g., while loop, early exits) and regular data (arrays with affine accesses).
- Design tiling schemes for modular dataflow programs: What does it mean to tile a dataflow program? Which compiler algorithms to use?
- Implement a mature compiler infrastructure from the front-end to code generation for a reasonable subset of the representation.

3.4. HLS-specific Dataflow Optimizations

The compiler analyses proposed in section 3.3 do not target a specific platform. In this part, we propose to leverage these analysis to develop source-level optimizations for high-level synthesis (HLS).

High-level synthesis consists in compiling a kernel written in a high-level language (typically in C) into a circuit. As for any compiler, an HLS tool consists in a *front-end* which translates the input kernel into an *intermediate representation*. This intermediate representation captures the control/flow dependences between computation units, generally in a hierarchical fashion. Then, the *back-end* maps this intermediate representation to a circuit (e.g. FPGA configuration). We believe that HLS tools must be thought as fine-grain automatic parallelizers. In classic HLS tools, the parallelism is expressed and exploited at the back-end level during the scheduling and the resource allocation of arithmetic operations. We believe that it would be far more profitable to derive the parallelism at the front-end level.

Hence, CASH will focus on the *front-end* pass and the *intermediate representation*. Low-level *back-end* techniques are not in the scope of CASH. Specifically, CASH will leverage the dataflow representation developed in Section 3.1 and the compilation techniques developed in Section 3.3 to develop a relevant intermediate representation for HLS and the corresponding front-end compilation algorithms.

Our results will be evaluated by using existing HLS tools (e.g., Intel HLS compiler, Xilinx Vivado HLS). We will implement our compiler as a source-to-source transformation in front of HLS tools. With this approach, HLS tools are considered as a "back-end black box". The CASH scheme is thus: (i) *front-end*: produce the CASH dataflow representation from the input C kernel. Then, (ii) turn this dataflow representation to a C program with pragmas for an HLS tool. This step must convey the characteristics of the dataflow representation found by step (i) (e.g. dataflow execution, fifo synchronisation, channel size). This source-to-source approach will allow us to get a full source-to-FPGA flow demonstrating the benefits of our tools while relying on existing tools for low-level optimizations. Step (i) will start from the DCC tool developed by Christophe Alias, which already produces a dataflow intermediate representation: the Data-aware Process Networks (DPN) [17]. Hence, the very first step is then to chose an HLS tool and to investiguate which input should be fed to the HLS tool so it "respects" the parallelism and the resource allocation suggested by the DPN. From this basis, we plan to investiguate the points described thereafter.

Roofline model and dataflow-level resource evaluation. Operational intensity must be tuned according to the roofline model. The roofline model [56] must be redefined in light of FPGA constraints. Indeed, the peak performance is no longer constant: it depends on the operational intensity itself. The more operational intensity we need, the more local memory we use, the less parallelization we get (since FPGA resources are limited), and finally the less performance we get! Hence, multiple iterations may be needed before reaching an efficient implementation. To accelerate the design process, we propose to iterate at the dataflow program level, which implies a fast resource evaluation at the dataflow level.

Reducing FPGA resources. Each parallel unit must use as little resources as possible to maximize parallel duplication, hence the final performance. This requires to factorize the control and the channels. Both can be achieved with source-to-source optimizations at dataflow level. The main issue with outputs from polyhedral optimization is large piecewise affine functions that require a wide silicon surface on the FPGA to be computed. Actually we do not need to compute a closed form (expression that can be evaluated in bounded time on the FPGA) *statically*. We believe that the circuit can be compacted if we allow control parts to be evaluated dynamically. Finally, though dataflow architectures are a natural candidate, adjustments are required to fit FPGA constraints (2D circuit, few memory blocks). Ideas from systolic arrays [48] can be borrowed to re-use the same piece of data multiple times, despite the limitation to regular kernels and the lack of I/O flexibility. A trade-off must be found between pure dataflow and systolic communications.

Improving circuit throughput. Since we target streaming applications, the throughput must be optimized. To achieve such an optimization, we need to address the following questions. How to derive an optimal upper bound on the throughput for polyhedral process network? Which dataflow transformations should be performed to reach it? The limiting factors are well known: I/O (decoding of burst data), communications through addressable channels, and latencies of the arithmetic operators. Finally, it is also necessary to find the right methodology to measure the throughput statically and/or dynamically.

3.4.1. Expected Impact

So far, the HLS front-end applies basic loop optimizations (unrolling, flattening, pipelining, etc.) and use a Hierarchical Control Flow Graph-like representation with data dependencies annotations (HCDFG). With this approach, we intend to demonstrate that polyhedral analysis combined with dataflow representations is an effective solution for HLS tools.

3.4.2. Scientific Program

3.4.2.1. Short-term and ongoing activities.

The HLS compiler designed in the CASH team currently extracts a fine-grain parallel intermediate representation (DPN [17], [16]) from a sequential program. We will not write a back-end that produces code for FPGA but we need to provide C programs that can be fed into existing C-to-FPGA compilers. However we obviously need an end-to-end compiler for our experiments. One of the first task of our HLS activity is to develop a DPN-to-C code generator suitable as input to an existing HLS tool like Vivado HLS. The generated code should exhibit the parallelism extracted by our compiler, and allow generating a final circuit more efficient than

the one that would be generated by our target HLS tool if ran directly on the input program. Source-to-source approaches have already been experimented successfully, e.g. in Alexandru Plesco's PhD [45].

3.4.2.2. Medium-term activities.

Our DPN-to-C code generation will need to be improved in many directions. The first point is the elimination of redundancies induced by the DPN model itself: buffers are duplicated to allow parallel reads, processes are produced from statements in the same loop, hence with the same control automaton. Also, multiplexing uses affine constraints which can be factorized [18]. We plan to study how these constructs can be factorized at C-level and to design the appropriate DPN-to-C translation algorithms.

Also, we plan to explore how on-the-fly evaluation can reduce the complexity of the control. A good starting point is the control required for the load process (which fetch data from the distant memory). If we want to avoid multiple load of the same data, the FSM (Finite State Machine) that describes it is usually very complex. We believe that dynamic construction of the load set (set of data to load from the main memory) will use less silicon than an FSM with large piecewise affine functions computed statically.

3.4.2.3. Long-term activities.

The DPN-to-C compiler will open new research perspectives. We will explore the roofline model accuracy for different applications by playing on DPN parameters (tile size). Unlike the classical roofline model, the peak performance is no longer assumed to be constant, but decreasing with operational intensity [58]. Hence, we expect a *unique* optimal set of parameters. Thus, we will build a DPN-level cost model to derive an interval containing the optimal parameters.

Also, we want to develop DPN-level analysis and transformation to quantify the optimal reachable throughput and to reach it. We expect the parallelism to increase the throughput, but in turn it may require an operational intensity beyond the optimal point discussed in the first paragraph. We will assess the trade-offs, build the cost-models, and the relevant dataflow transformations.

3.5. Simulation of Hardware

Complex systems such as systems-on-a-chip or HPC computer with FPGA accelerator comprise both hardware and software parts, tightly coupled together. In particular, the software cannot be executed without the hardware, or at least a simulator of the hardware.

Because of the increasing complexity of both software and hardware, traditional simulation techniques (Register Transfer Level, RTL) are too slow to allow full system simulation in reasonable time. New techniques such as Transaction Level Modeling (TLM) [14] in SystemC [13] have been introduced and widely adopted in the industry. Internally, SystemC uses discrete-event simulation, with efficient context-switch using cooperative scheduling. TLM abstracts away communication details, and allows modules to communicate using function calls. We are particularly interested in the loosely timed coding style where the timing of the platform is not modeled precisely, and which allows the fastest simulations. This allowed gaining several orders of magnitude of simulation speed. However, SystemC/TLM is also reaching its limits in terms of performance, in particular due to its lack of parallelism.

Work on SystemC/TLM parallel execution is both an application of other work on parallelism in the team and a tool complementary to HLS presented in Sections 3.1 (dataflow models and programs) and 3.4 (application to FPGA). Indeed, some of the parallelization techniques we develop in CASH could apply to SystemC/TLM programs. Conversely, a complete design-flow based on HLS needs fast system-level simulation: the full-system usually contains both hardware parts designed using HLS, handwritten hardware components, and software.

We will also work on simulation of the DPN intermediate representation. Simulation is a very important tool to help validate and debug a complete compiler chain. Without simulation, validating the front-end of the compiler requires running the full back-end and checking the generated circuit. Simulation can avoid the execution time of the backend and provide better debugging tools.

Automatic parallelization has shown to be hard, if at all possible, on loosely timed models [23]. We focus on semi-automatic approaches where the programmer only needs to make minor modifications of programs to get significant speedups.

3.5.1. Expected Impact

The short term impact is the possibility to improve simulation speed with a reasonable additional programming effort. The amount of additional programming effort will thus be evaluated in the short term.

In the longer term, our work will allow scaling up simulations both in terms of models and execution platforms. Models are needed not only for individual Systems on a Chip, but also for sets of systems communicating together (e.g., the full model for a car which comprises several systems communicating together), and/or heterogeneous models. In terms of execution platform, we are studying both parallel and distributed simulations.

3.5.2. Scientific Program

3.5.2.1. Short-term and ongoing activities.

We started the joint PhD (with Tanguy Sassolas) of Gabriel Busnot with CEA-LIST. The research targets parallelizing SystemC heterogeneous simulations. CEA-LIST already developed SCale [54], which is very efficient to simulate parallel homogeneous platforms such as multi-core chips. However, SCale cannot currently load-balance properly the computations when the platform contains different components modeled at various levels of abstraction. Also, SCale requires manual annotations to identify accesses to shared variables. These annotations are given as address ranges in the case of a shared memory. This annotation scheme does not work when the software does non-trivial memory management (virtual memory using a memory management unit, dynamic allocation), since the address ranges cannot be known statically. We started working on the "heterogeneous" aspect of simulations with an approach allowing changing the level of details in a simulation at runtime, and started tackling the virtual and dynamic memory management problem by porting Linux on our simulation platform.

We also started working on an improved support for simulation and debugging of the DPN internal representation of our parallelizing compiler (see Section 3.3). A previous quick experiment with simulation was to generate C code that simulates parallelism with POSIX-threads. While this simulator greatly helped debug the compiler, this is limited in several ways: simulations are not deterministic, and the simulator does not scale up since it would create a very large number of threads for a non-trivial design.

We are working in two directions. The first is to provide user-friendly tools to allow graphical inspection of traces. For example, we will work on the visualization of the sequence of steps leading to a deadlock when the situation occurs, and give hints on how to fix the problem in the compiler. The second is to use an efficient simulator to speed up the simulation. We plan to generate SystemC/TLM code from the DPN representation to benefit from the ability of SystemC to simulate a large number of processes.

3.5.2.2. Medium-term activities.

Several research teams have proposed different approaches to deal with parallelism and heterogeneity. Each approach targets a specific abstraction level and coding style. While we do not hope for a universal solution, we believe that a better coordination of different actors of the domain could lead to a better integration of solutions. We could imagine, for example, a platform with one subsystem accelerated with SCale [54] from CEA-LIST, some compute-intensive parts delegated to sc-during [43] from Matthieu Moy, and a co-simulation with external physical solvers using SystemC-MDVP [21] from LIP6. We plan to work on the convergence of approaches, ideally both through point-to-point collaborations and with a collaborative project.

A common issue with heterogeneous simulation is the level of abstraction. Physical models only simulate one scenario and require concrete input values, while TLM models are usually abstract and not aware of precise physical values. One option we would like to investigate is a way to deal with loose information, e.g. manipulate intervals of possible values instead of individual, concrete values. This would allow a simulation to be symbolic with respect to the physical values.

Obviously, works on parallel execution of simulations would benefit to simulation of data-aware process networks (DPN). Since DPN are generated, we can even tweak the generator to guarantee some properties on the generated code, which will give us more freedom on the parallelization and partitioning techniques.

3.5.2.3. Long-term activities.

In the long term, our vision is a simulation framework that will allow combining several simulators (not necessarily all SystemC-based), and allow running them in a parallel way. The Functional Mockup Interface (FMI) standard is a good basis to build upon, but the standard does not allow expressing timing and functional constraints needed for a full co-simulation to run properly.

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 [5] 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*) [55], 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 [41], 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 general purpose but also for domain specific 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 run-time 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, run-time 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); Run-time 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 run-time 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 run-time 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.

DATASPHERE Team

3. Research Program

3.1. Dynamics of digital transformations

The research program of the Datasphere team aims at understanding the transformations induced by digital systems on socio-economic and socio-ecological organizations. These transformations are very broad and impact a large part of society. Understanding these changes is very ambitious and would require much more resources than those of the team. Interactions with other teams in other disciplines is thus of strategic importance. The research directions we have worked in and will continue to in the coming years are the following.

- The legal and strategic implications of the development of networks, the growing global interdependencies, and the increase of digital flows beyond control.
- The geopolitics of digital systems, data flows and cyber control, the raise of new strategic imbalances, and digital powers (US, China, Russia, etc.)
- The structural consequences of the translation of governance to digital actors, their inclusion into diplomatic forums, and the weakening of sovereignty over territories.

3.2. Foundations of digital economy

- The economy of intermediation and the progressive control of all two-sided and multi-sided markets by remote digital platforms.
- The methodologies for assessing the strategic value of data and evaluating its leverage for the political economy.
- The analysis of Online Advertisement/tracking ecosystems.

3.3. Ecosystems and Anthropocene

- The interdependencies of natural ecosystems and socio-economic systems, and the role of digital systems on measuring and controlling the global natural/social system.
- The role of digital actors in the adaptation and mitigation of climate change.
- The information economy of planetary challenges related to global warming, biodiversity, health monitoring.

3.4. Large scale graph analysis

- Community analysis and extraction, spectral methods.
- Manifold based approaches to large scale graph analysis, optimal transport.
- Information/rumor/fake news propagation in social networks.

PRIVATICS Project-Team (section vide)

SPADES Project-Team

3. Research Program

3.1. Introduction

The SPADES research program is organized around three main themes, *Design and Programming Models*, *Certified real-time programming*, and *Fault management and causal analysis*, 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. Design and Programming Models

Work on this theme aims to develop models , languages and tools to support a "correct-by-construction" approach to the development of embedded systems.

On the programming side, we focus on the definition of domain specific programming models and languages supporting static analyses for the computation of precise resource bounds for program executions. We propose dataflow models supporting dynamicity while enjoying effective analyses. In particular, we study parametric extensions where properties such as liveness and boundedness remain statically analyzable.

On the design side, we focus on the definition of component-based models for software architectures combining distribution, dynamicity, real-time and fault-tolerant aspects. Component-based construction has long been advocated as a key approach to the "correct-by-construction" design of complex embedded systems [49]. Witness component-based toolsets such as PTOLEMY [38], BIP [30], or the modular architecture frameworks used, for instance, in the automotive industry (AUTOSAR) [22]. 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.

Formal models for component-based design are an active area of research. 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).

We plan to develop our component theory by progressing on two fronts: a semantical framework and domain-specific programming models. 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 first main objective for this axis.

3.3. Certified Real-Time 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 [32]), 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 [28], [36], 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. [28]. For our part, we intend to focus on devising synchronous programming languages for distributed systems and precision-timed architectures.

3.4. Fault Management and Causal Analysis

Managing faults is a clear and present necessity in networked embedded systems. At the hardware level, modern multicore architectures are manufactured using inherently unreliable technologies [33], [43]. 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.

In this axis we intend to address the question of *how to cope with faults and failures in embedded systems?*. We will tackle this question by exploiting reversible programming models and by developing techniques for fault ascription and explanation in component-based systems.

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 [53], natural sciences, law [54], and statistics [55], 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 [52], to allow the diagnosis of faults in a complex concurrent system [47], or to enforce accountability [51], 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 [45]), or is broken (*e.g.*, by limiting fault propagation [57]).

ELAN Team

3. Research Program

3.1. Discrete modeling of slender elastic structures

For the last 15 years, we have investigated new discrete models for solving the Kirchhoff dynamic equations for thin elastic rods [7], [9], [12]. All our models share a curvature-based spatial discretization, allowing them to capture inextensibility of the rod intrinsically, without the need for adding any kinematic constraint. Moreover, elastic forces boil down to linear terms in the dynamic equations, making them well-suited for implicit integration. Interestingly, our discretization methodology can be interpreted from two different points-of-views. From the finite-elements point-of-view, our strain-based discrete schemes can be seen as discontinuous Galerkin methods of zero and first orders. From the multibody system dynamics point of view, our discrete models can be interpreted as deformable Lagrangian systems in finite dimension, for which a dedicated community has started to grow recently [33]. We note that adopting the multibody system dynamics point of view helped us formulate a linear-time integration scheme [8], which had only be investigated in the case of multibody rigid bodies dynamics so far.

3.1.1. High-order spatial discretization schemes for rods, ribbons and shells

Our goal is to investigate similar high-order modeling strategies for surfaces, in particular for the case of inextensible ribbons and shells. Elastic ribbons have been scarcely studied in the past, but they are nowadays drawing more and more the attention from physicists [22], [31]. Their numerical modeling remains an open challenge. In contrast to ribbons, a huge litterature exists for shells, both from a theoretical and numerical viewpoints (see, e.g., [26], [13]). However, no real consensus has been obtained so far about a unified nonlinear shell theory able to support large displacements. In [10] we have started building an inextensible shell patch by taking as degrees of freedom the curvatures of its mid-surface, expressed in the local frame. As in the super-helix model, we show that when taking curvatures uniform over the element, each term of the equations of motion may be computed in closed-form; besides, the geometry of the element corresponds to a cylinder patch at each time step. Compared to the 1D (rod) case however, some difficulties arise in the 2D (plate/shell) case, where compatibility conditions are to be treated carefully.

3.1.2. Numerical continuation of rod equilibria in the presence of unilateral constraints

In Alejandro Blumentals' PhD thesis [11], we have adopted an optimal control point of view on the static problem of thin elastic rods, and we have shown that direct discretization methods [0] are particularly well-suited for dealing with scenarios involving both bilateral and unilateral constraints (such as contact). We would like to investigate how our formulations extend to continuation problems, where the goal is to follow a certain branch of equilibria when the rod is subject to some varying constraints (such as one fixed end being applied a constant rotation). To the best of our knowledge, classical continuation methods used for rods [23] are not able to deal with non-persistent or sliding contact.

3.2. Discrete modeling of frictional contact

Most popular approaches in Computer Graphics and Mechanical Engineering consist in assuming that the objects in contact are locally compliant, allowing them to slightly penetrate each other. This is the principle of penalty-based methods (or molecular dynamics), which consists in adding mutual repulsive forces of the form $k\,f(\delta)$, where δ is the penetration depth detected at current time step [14], [30]. Though simple to implement and computationally efficient, the penalty-based method often fails to prevent excessive penetration of the contacting objects, which may prove fatal in the case of thin objects as those may just end up traversing each other. One solution might be to set the stiffness factor k to a large enough value, however this causes the introduction of parasitical high frequencies and calls for very small integration steps [6]. Penalty-based approaches are thus generally not satisfying for ensuring robust contact handling.

[0] Within this optimal control framework, our previous curvature-based methods can actually be interpreted as a special case of direct single shooting methods.

In the same vein, the friction law between solid objects, or within a yield-stress fluid (used to model foam, sand, or cement, which, unlike water, cannot flow beyond a certain threshold), is commonly modeled using a regularized friction law (sometimes even with simple viscous forces), for the sake of simplicity and numerical tractability (see e.g., [32], [25]). Such a model cannot capture the threshold effect that characterizes friction between contacting solids or within a yield-stress fluid. The nonsmooth transition between sticking and sliding is however responsible for significant visual features, such as the complex patterns resting on the outer surface of hair, the stable formation of sand piles, or typical stick-slip instabilities occurring during motion.

The search for a realistic, robust and stable frictional contact method encouraged us to depart from those, and instead to focus on rigid contact models coupled to the exact nonsmooth Coulomb law for friction (and respectively, to the exact nonsmooth Drucker-Prager law in the case of a fluid), which better integrate the effects of frictional contact at the macroscopic scale. This motivation was the sense of the hiring of F. Bertails-Descoubes in 2007 in the Inria/LJK BIPOP team, specialized in nonsmooth mechanics and related convex optimization methods. In the line of F. Bertails-Descoubes's work performed in the BIPOP team, the ELAN team keeps on including some active research on the finding of robust frictional contact algorithms specialized for slender deformable structures.

3.2.1. Optimized algorithms for large nodal systems in frictional contact

In the fiber assembly case, the resulting mass matrix M is block-diagonal, so that the Delassus operator can be computed in an efficient way by leveraging sparse-block computations [15]. This justifies solving the reduced discrete frictional contact problem where primary unknowns are forces, as usually advocated in nonsmooth mechanics [28]. For cloth however, where primal variables (nodal velocities of the cloth mesh) are all interconnected via elasticity through implicit forces, the method developed above is computationally inefficient. Indeed, the matrix M (only block-sparse, but not block-diagonal) is costly to invert for large systems and its inverse is dense. Recently, we have leveraged the fact that generalized velocities of the system are 3D velocities, which simplifies the discrete contact problem when contacts occur at the nodes. Combined with a multiresolution strategy, we have devised an algorithm able to capture exact Coulomb friction constraints at contact, while retaining computational efficiency [29]. This work also supports cloth self-contact and cloth multilayering. How to enrich the interaction model with, e.g., cohesion, remains an open question. The experimental validation of our frictional contact model is also one of our goals in the medium run.

3.2.2. Continuum modeling of large fiber assemblies

Though we have recently made progress on the continuum formulation and solving of granular materials in Gilles Daviet's PhD thesis [19], [17], [16], we are still far from a continuum description of a macroscopic dry fibrous medium such as hair. One key ingredient that we have not been considering in our previous models is the influence of air inside divided materials. Typically, air plays a considerable role in hair motion. To advance in that direction, we have started to look at a diphasic fluid representation of granular matter, where a Newtonian fluid and the solid phase are fully coupled, while the nonsmooth Drucker-Prager rheology for the solid phase is enforced implicitly [18]. This first approach could be a starting point for modeling immersed granulars in a liquid, or ash clouds, for instance.

A long path then remains to be achieved, if one wants to take into account long fibers instead of isotropic grains in the solid phase. How to couple the fiber elasticity with our current formulation remains a challenging problem.

3.3. Inverse design of slender elastic structures [ERC Gem]

With the considerable advance of automatic image-based capture in Computer Vision and Computer Graphics these latest years, it becomes now affordable to acquire quickly and precisely the full 3D geometry of many mechanical objects featuring intricate shapes. Yet, while more and more geometrical data get collected and shared among the communities, there is currently very little study about how to infer the underlying mechanical properties of the captured objects merely from their geometrical configurations.

An important challenge consists in developing a non-invasive method for inferring the mechanical properties of complex objects from a minimal set of geometrical poses, in order to predict their dynamics. In contrast to classical inverse reconstruction methods, our claim is that 1/ the mere geometrical shape of physical objects reveals a lot about their underlying mechanical properties and 2/ this property can be fully leveraged for a wide range of objects featuring rich geometrical configurations, such as slender structures subject to contact and friction (e.g., folded cloth or twined filaments).

In addition to significant advances in fast image-based measurement of diverse mechanical materials stemming from physics, biology, or manufacturing, this research is expected in the long run to ease considerably the design of physically realistic virtual worlds, as well as to boost the creation of dynamic human doubles.

To achieve this goal, we shall develop an original inverse modeling strategy based upon the following research topics:

3.3.1. Design of well-suited discrete models for slender structures

We believe that the quality of the upstream, reference physics-based model is essential to the effective connection between geometry and mechanics. Typically, such a model should properly account for the nonlinearities due to large displacements of the structures, as well as to the nonsmooth effects typical of contact and friction.

It should also be parameterized and discretized in such a way that inversion gets simplified mathematically, possibly avoiding the huge cost of large and nonconvex optimization. In that sense, unlike concurrent methods which impose inverse methods to be compatible with a generic physics-based model, we instead advocate the design of specific physics-based models which are tailored for the inversion process.

More precisely, from our experience on fiber modeling, we believe that reduced Lagrangian models, based on a minimal set of coordinates and physical parameters (as opposed to maximal coordinates models such as mass-springs), are particularly well-suited for inversion and physical interpretation of geometrical data [21], [20]. Furthermore, choosing a high-order coordinate system (e.g., curvatures instead of angles) allows for a precise handling of curved boundaries and contact geometry, as well as the simplification of constitutive laws (which are transformed into a linear equation in the case of rods). We are currently investigating high-order discretization schemes for elastic ribbons and developable shells [10].

3.3.2. Static inversion of physical objects from geometrical poses

We believe that pure static inversion may by itself reveal many insights regarding a range of parameters such as the undeformed configuration of the object, some material parameters or contact forces.

The typical settings that we consider is composed of, on the one hand, a reference mechanical model of the object of interest, and on the other hand a single or a series of complete geometrical poses corresponding each to a static equilibrium. The core challenge consists in analyzing theoretically and practically the amount of information that can be gained from one or several geometrical poses, and to understand how the fundamental under-determinacy of the inverse problem can be reduced, for each unknown quantity (parameter or force) at play. Both the equilibrium condition and the stability criterion of the equilibrium are leveraged towards this goal. On the theoretical side, we have recently shown that a given 3D curve always matches the centerline of an isotropic suspended Kirchhoff rod at equilibrium under gravity, and that the natural configuration of the rod is unique once material parameters (mass, Young modulus) are fixed [1]. On the practical side, we have recently devised a robust algorithm to find a valid natural configuration for a discrete shell to match a given surface under gravity and frictional contact forces [3]. Unlike rods however, shells can have multiple inverse (natural) configurations. Choosing among the multiple solutions based on some selection criteria is an open challenge. Another open issue, in all cases, is the theoretical characterization of material parameters allowing the equilibrium to be stable.

3.3.3. Dynamic inversion of physical objects from geometrical poses

To refine the solution subspaces searched for in the static case and estimate dynamic parameters (e.g., some damping coefficients), a dynamic inversion process accounting for the motion of the object of interest is necessary.

In contrast to the static case where we can afford to rely on exact geometrical poses, our analysis in the dynamic case will have to take into account the imperfect quality of input data with possible missing parts or outliers. One interesting challenge will be to combine our high-order discretized physics-based model together with the acquisition process in order to refine both the parameter estimation and the geometrical acquisition.

3.3.4. Experimental validation with respect to real data

The goal will be to confront the theories developed above to real experiments. Compared to the statics, the dynamic case will be particularly involving as it will be highly dependent on the quality of input data as well as the accuracy of the motion predicted by our physics-based simulators. Such experiments will not only serve to refine our direct and inverse models, but will also be leveraged to improve the 3D geometrical acquisition of moving objects. Besides, once validation will be performed, we shall work on the setting up of new non-invasive measurement protocols to acquire physical parameters of slender structures from a minimal amount of geometrical configurations.

MISTIS Project-Team

3. Research Program

3.1. Mixture models

Participants: Alexis Arnaud, Jean-Baptiste Durand, Florence Forbes, Stéphane Girard, Julyan Arbel, Jean-Michel Bécu, Hongliang Lu, Fabien Boux, Veronica Munoz Ramirez, Benoit Kugler, Alexandre Constantin, Fei Zheng.

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,

$$f(y_i; \theta) = \sum_{k=1}^{K} P(z_i = k; \theta) f(y_i \mid z_i; \theta) \ . \tag{1}$$

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: Alexis Arnaud, Brice Olivier, Thibaud Rahier, Jean-Baptiste Durand, Florence Forbes, Karina Ashurbekova, Hongliang Lu, Pierre-Antoine Rodesch, Julyan Arbel, Mariia Vladimirova.

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: Clément Albert, Stéphane Girard, Florence Forbes, Jean-Michel Bécu, Antoine Usseglio Carleve, Pascal Dkengne Sielenou, Marta Crispino, Meryem Bousebata.

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 [79] 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).

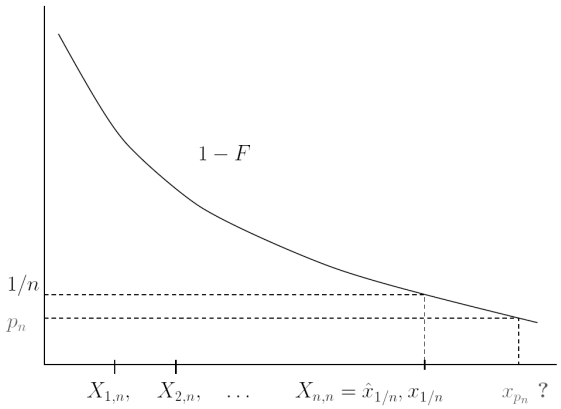


Figure 1. The curve represents the survival function $x \to P(X > x)$. The $1/n$-quantile is estimated by the maximum observation so that $\widehat{x}_{1/n} = X_{n,n}$. As illustrated in the figure, to estimate p_n-quantiles with $p_n < 1/n$, it is necessary to extrapolate beyond the maximum observation.

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:

$$P(X > x) = x^{-1/\theta}\ell(x),\ x > x_0 > 0, \tag{2}$$

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

$$\frac{\ell(tx)}{\ell(x)} \to 1 \text{ as } x \to \infty \tag{3}$$

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:

$$P(X > x) = \exp\{-x^{\theta}\ell(x)\},\ x > x_0 > 0. \tag{4}$$

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 distortions 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 [75]. 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 [79].

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 [79].

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 [49]. 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 [50], a wheelbarrow molecule [60], a nano-car [83], a Morse molecule [33], etc. Typically, these designs are optimized using semi-empirical quantum mechanics calculations, such as the semi-empirical ASED+ calculation technique [34].

While impressive, these are but two examples of the nanoscience revolution already impacting numerous fields, including electronics and semiconductors [64], textiles [63], [54], energy [69], food [44], drug delivery [52], [85], chemicals [55], materials [45], the automotive industry [31], aerospace and defense [51], medical devices and therapeutics [47], medical diagnostics [86], etc. According to some estimates, the world market for nanotechnology-related products and services will reach one trillion dollars by 2015 [78]. 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 [89], removing some degrees of freedom (e.g. keeping torsion angles only [62], [84]), coarse-graining [87], [81], [35], [82], multiple time step methods [75], [76], fast multipole methods [48], parallelization [61], averaging [43], multi-scale modeling [42], [39], reactive force fields [41], [92], interactive multiplayer games for predicting protein structures [46], 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 [90], [91].

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 [71], [72], [73], [74], the adaptive multiscale method [68], and the adaptive partitioning of the Lagrangian method [56]. 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. As-Rigid-As-Possible methods for molecular paths

Last year, in the scope of Minh Khoa Nguyen's PhD, we have adapted the As-Rigid-As-Possible (ARAP) paradigm used in Computer Graphics to generate paths of molecular systems. This year, we continued this line of research with new extensions of the ARAP methodology. One extension led to generate conformational transition paths with low potential-energy barriers for proteins. It was published to the Journal of Computer-Aided Molecular Design, 2018 [66]. Another extension concerned the ART-RRT method which incorporates the ARAP methodology inside tree-based exploration methods to approximate ligand unbinding pathways. This contribution was published to the Journal of Computational Chemistry, 2018 [65]. Finally, the PhD thesis of Minh Khoa Nguyen titled *Efficient exploration of molecular paths from As-Rigid-As-Possible approaches and motion planning methods* was defended in March 2018 [67]. A brief summary of the above-mentioned contributions is presented below.

3.5. Modelling and simulation for the characterization of advanced materials

We have continued our informal collaboration with the *service de Caractérisation des Matériaux et Composants* of CEA, LETI, Minatec initiated in 2017. The collaboration with LETI will offer numerous possibilities of very precise (sub-nanometric) experimental comparisons based on the High-resolution scanning transmission electron microscopy (HRSTEM) using one of the best microscopes on the market (the FEI Titan Ultimate microscope). In this context, we have developed a set of tools tools to manipulate, simulate and measure nanomaterials, with a special focus on crystals that appears in many new materials such as semiconductors. The description of the sublines of research explored so far are detailed below.

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.
- 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 identified before (e.g., decentralized/collaborative traffic optimal control, density balancing using consensus concepts, data fusion, distributed estimation, etc.). Several specific actions have been continued/launched to this purpose: improvement and finalization of the Grenoble Traffic Lab(GTL), EU projects (SPEEDD, ERC-AdG Scale-FreeBack). Further research goals are envisioned, such as:

- Modeling of large scale traffic systems. We aim at reducing the complexity of traffic systems modeling by engaging novel modeling techniques that make use of clustering for traffic networks while relying on its specific characteristics. Traffic networks will be aggregate into clusters and the main traffic quantities will be extrapolated by making use of this aggregation. Moreover, we are developing an extension of the Grenoble Traffic Lab (GTL) for downtown Grenoble which will make use of GPS and probe data to collect traffic data in the city center.
- Modeling and control of intelligent transportation systems. We aim at developing a complete micro-macro modeling approach to describe and model the new traffic dynamics that is developing thanks to mixed (simple, connected and automated) vehicles in the roads. This will require cutting edge mathematical theory and field experiments.

TRIPOP Team

3. Research Program

3.1. Introduction

In this section, we develop our scientific program. In the framework of nonsmooth dynamical systems, the activities of the project–team will be on focused on the following research axes:

- *Axis 1: Modeling and analysis (detailed in Sect. 3.2).*
- *Axis 2: Numerical methods and simulation (detailed in Sect. 3.3).*
- *Axis 3: Automatic Control (detailed in Sect. 3.4)*

These research axes will be developed with a strong emphasis on the software development and the industrial transfer that are detailed respectively in Sect. 5.1 and Sect. 7.1 .

3.2. Axis 1: Modeling and analysis

This axis is dedicated to the modeling and the mathematical analysis of nonsmooth dynamical systems. It consists of four main directions. Two directions are in the continuation of BIPOP activities: 1) multibody vibro-impact systems (Sect. 3.2.1) and 2) excitable systems (Sect. 3.2.2). Two directions are completely new with respect to BIPOP: 3) Nonsmooth geomechanics and natural hazards assessment (Sect. 3.2.3) and 4) Cyber-physical systems (hybrid systems) (Sect. 3.2.4).

3.2.1. Multibody vibro-impact systems

Participants: B. Brogliato, F. Bourrier, G. James, V. Acary

- *Multiple impacts with or without friction :* there are many different approaches to model collisions, especially simultaneous impacts (so-called multiple impacts) [84]. One of our objectives is on one hand to determine the range of application of the models (for instance, when can one use "simplified" rigid contact models relying on kinematic, kinetic or energetic coefficients of restitution?) on typical benchmark examples (chains of aligned beads, rocking block systems). On the other hand, try to take advantage of the new results on nonlinear waves phenomena, to better understand multiple impacts in 2D and 3D granular systems. The study of multiple impacts with (unilateral) nonlinear visco-elastic models (Simon-Hunt-Crossley, Kuwabara-Kono), or visco-elasto-plastic models (assemblies of springs, dashpots and dry friction elements), is also a topic of interest, since these models are widely used.
- *Artificial or manufactured or ordered granular crystals, meta-materials :* Granular metamaterials (or more general nonlinear mechanical metamaterials) offer many perspectives for the passive control of waves originating from impacts or vibrations. The analysis of waves in such systems is delicate due to spatial discreteness, nonlinearity and non-smoothness of contact laws [86], [72], [73], [79]. We will use a variety of approaches, both theoretical (e.g. bifurcation theory, modulation equations) and numerical, in order to describe nonlinear waves in such systems, with special emphasis on energy localization phenomena (excitation of solitary waves, fronts, breathers).
- *Systems with clearances, modeling of friction :* joint clearances in kinematic chains deserve specific analysis, especially concerning friction modeling [40]. Indeed contacts in joints are often conformal, which involve large contact surfaces between bodies. Lubrication models should also be investigated.
- *Painlevé paradoxes :* the goal is to extend the results in [65], which deal with single-contact systems, to multi-contact systems. One central difficulty here is the understanding and the analysis of singularities that may occur in sliding regimes of motion.

As a continuation of the work in the BIPOP team, our software code, Siconos (see Sect. 5.1) will be our favorite software platform for the integration of these new modeling results.

3.2.2. Excitable systems

Participants: A. Tonnelier, G. James

An excitable system elicits a strong response when the applied perturbation is greater than a threshold [81], [82], [45], [91]. This property has been clearly identified in numerous natural and physical systems. In mechanical systems, non-monotonic friction law (of spinodal-type) leads to excitability. Similar behavior may be found in electrical systems such as active compounds of neuristor type. Models of excitable systems incorporate strong non-linearities that can be captured by non-smooth dynamical systems. Two properties are deeply associated with excitable systems: oscillations and propagation of nonlinear waves (autowaves in coupled excitable systems). We aim at understanding these two dynamical states in excitable systems through theoretical analysis and numerical simulations. Specifically we plan to study:

- Threshold-like models in biology: spiking neurons, gene networks.
- Frictional contact oscillators (slider block, Burridge-Knopoff model).
- Dynamics of active electrical devices : memristors, neuristors.

3.2.3. Nonsmooth geomechanics and natural hazards assessment

Participants: F. Bourrier, B. Brogliato, G. James, V. Acary

- *Rockfall impact modeling :* Trajectory analysis of falling rocks during rockfall events is limited by a rough modeling of the impact phase [47], [46], [77]. The goal of this work is to better understand the link between local impact laws at contact with refined geometries and the efficient impact laws written for a point mass with a full reset map. A continuum of models in terms of accuracy and complexity will be also developed for the trajectory studies. In particular, nonsmooth models of rolling friction, or rolling resistance will be developed and formulated using optimization problems.
- *Experimental validation :* The participation of IRSTEA with F. Bourrier makes possible the experimental validation of models and simulations through comparisons with real data. IRSTEA has a large experience of lab and in-situ experiments for rockfall trajectories modeling [47], [46]. It is a unique opportunity to vstrengthen our model and to prove that nonsmooth modeling of impacts is reliable for such experiments and forecast of natural hazards.
- *Rock fracturing :* When a rock falls from a steep cliff, it stores a large amount of kinetic energy that is partly dissipated though the impact with the ground. If the ground is composed of rocks and the kinetic energy is sufficiently high, the probability of the fracture of the rock is high and yields an extra amount of dissipated energy but also an increase of the number of blocks that fall. In this item, we want to use the capability of the nonsmooth dynamical framework for modeling cohesion and fracture [74], [38] to propose new impact models.
- *Rock/forest interaction :* To prevent damages and incidents to infrastructures, a smart use of the forest is one of the ways to control trajectories (decrease of the run-out distance, jump heights and the energy) of the rocks that fall under gravity [58], [59]. From the modeling point of view and to be able to improve the protective function of the forest, an accurate modeling of impacts between rocks and trees is required. Due to the aspect ratio of the trees, they must be considered as flexible bodies that may be damaged by the impact. This new aspect offers interesting modeling research perspectives.

More generally, our collaboration with IRSTEA opens new long term perspectives on granular flows applications such as debris and mud flows, granular avalanches and the design of structural protections. *The numerical methods that go with these new modeling approaches will be implemented in our software code, Siconos (see Sect. 5.1)*

3.2.4. Cyber-physical systems (hybrid systems)

Participants: V. Acary, B. Brogliato, C. Prieur, A. Tonnelier

Nonsmooth systems have a non-empty intersection with hybrid systems and cyber–physical systems. However, nonsmooth systems enjoy strong mathematical properties (concept of solutions, existence and uniqueness) and efficient numerical tools. This is often the result of the fact that nonsmooth dynamical systems are models of physical systems, and then, take advantage of their intrinsic property (conservation or dissipation of energy, passivity, stability). A standard example is a circuit with n ideal diodes. From the hybrid point of view, this circuit is a piecewise smooth dynamical system with 2^n modes, that can be quite cumbersome to enumerate in order to determinate the current mode. As a nonsmooth system, this circuit can be formulated as a complementarity system for which there exist efficient time–stepping schemes and polynomial time algorithms for the computation of the current mode. The key idea of this research action is to take benefit of this observation to improve the hybrid system modeling tools.

Research actions: There are two main actions in this research direction that will be implemented in the framework of the Inria Project Lab (IPL " Modeliscale", see https://team.inria.fr/modeliscale/ for partners and details of the research program):

•*Structural analysis of multimode DAE :* When a hybrid system is described by a Differential Algebraic Equation (DAE) with different differential indices in each continuous mode, the structural analysis has to be completely rethought. In particular, the re-initialization rule, when a switching occurs from a mode to another one, has to be consistently designed. We propose in this action to use our knowledge in complementarity and (distribution) differential inclusions [33] to design consistent re-initialization rule for systems with nonuniform relative degree vector $(r_1, r_2, ..., r_m)$ and $r_i \neq r_j, i \neq j$.

•*Cyber–physical in hybrid systems modeling languages :* Nowadays, some hybrid modeling languages and tools are widely used to describe and to simulate hybrid systems (MODELICA, SIMULINK, and see [55] for references therein). Nevertheless, the compilers and the simulation engines behind these languages and tools suffer from several serious weaknesses (failure, weird output or huge sensitivity to simulation parameters), especially when some components, that are standard in nonsmooth dynamics, are introduced (piecewise smooth characteristic, unilateral constraints and complementarity condition, relay characteristic, saturation, dead zone, ...). One of the main reasons is the fact that most of the compilers reduce the hybrid system to a set of smooth modes modeled by differential algebraic equations and some guards and reinitialization rules between these modes. Sliding mode and Zeno–behaviour are really harsh for hybrid systems and relatively simple for nonsmooth systems. With B. Caillaud (Inria HYCOMES) and M. Pouzet (Inria PARKAS), we propose to improve this situation by implementing a module able to identify/describe nonsmooth elements and to efficiently handle them with SICONOS as the simulation engine. They have already carried out a first implementation [53] in Zelus, a synchronous language for hybrid systems http://zelus.di.ens.fr. Removing the weaknesses related to the nonsmoothness of solutions should improve hybrid systems towards robustness and certification.

•*A general solver for piecewise smooth systems* This direction is the continuation of the promising result on modeling and the simulation of piecewise smooth systems [37]. As for general hybrid automata, the notion or concept of solutions is not rigorously defined from the mathematical point of view. For piecewise smooth systems, multiplicity of solutions can happen and sliding solutions are common. The objective is to recast general piecewise smooth systems in the framework of differential inclusions with Aizerman–Pyatnitskii extension [37], [61]. This operation provides a precise meaning to the concept of solutions. Starting from this point, the goal is to design and study an efficient numerical solver (time–integration scheme and optimization solver) based on an equivalent formulation as mixed complementarity systems of differential variational inequalities. We are currently discussing the issues in the mathematical analysis. The goal is to prove the convergence of the time–stepping scheme to get an existence theorem. With this work, we should also be able to discuss the general Lyapunov stability of stationary points of piecewise smooth systems.

3.3. Axis 2: Numerical methods and simulation

This axis is dedicated to the numerical methods and simulation for nonsmooth dynamical systems. As we mentioned in the introduction, the standard numerical methods have been largely improved in terms of accuracy and dissipation properties in the last decade. Nevertheless, the question of the geometric

time–integration techniques remains largely open. It constitutes the objective of the first research direction in Sect. 3.3.1 . Beside the standard IVP, the question of normal mode analysis for nonsmooth systems is also a research topic that emerged in the recent years. More generally, the goal of the second research direction (Sect. 3.3.2) is to develop numerical methods to solve boundary value problems in the nonsmooth framework. This will serve as a basis for the computation of the stability and numerical continuation of invariants. Finally, once the time-integration method is chosen, it remains to solve the one-step nonsmooth problem, which is, most of time, a numerical optimization problem. In Sect. 3.3.3 , we propose to study two specific problems with a lot of applications: the Mathematical Program with Equilibrium Constraints (MPEC) for optimal control, and Second Order Cone Complementarity Problems (SOCCP) for discrete frictional contact systems. After some possible prototypes in scripting languages (Python and Matlab), we will be attentive that all these developments of numerical methods will be integrated in Siconos.

3.3.1. Geometric time–integration schemes for nonsmooth Initial Value Problem (IVP)

Participants: V. Acary, B. Brogliato, G. James, F. Pérignon
The objective of this research item is to continue to improve classical time–stepping schemes for nonsmooth systems to ensure some qualitative properties in discrete-time. In particular, the following points will be developed

- Conservative and dissipative systems. The question of the energy conservation and the preservation of dissipativity properties in the Willems sense [64] will be pursued and extended to new kinds of systems (nonlinear mechanical systems with nonlinear potential energy, systems with limited differentiability (rigid impacts vs. compliant models)).
- Lie–group integration schemes for finite rotations for the multi-body systems extending recent progresses in that directions for smooth systems [43].
- Conservation and preservation of the dispersion properties of the (non)-dispersive system.

3.3.2. Stability and numerical continuation of invariants

Participants: G. James, V. Acary, A. Tonnelier, F. Pérignon,

By invariants, we mean equilibria, periodic solutions, limit cycles or waves. Our preliminary work on this subject raised the following research perspectives:

- Computation of periodic solutions of discrete mechanical systems . The modal analysis, *i.e.*, a spectral decomposition of the problem into linear normal modes is one of the basic tools for mechanical engineers to study dynamic response and resonance phenomena of an elastic structure. Since several years, the concept of nonlinear normal modes [75], that is closely related to the computation of quasi-periodic solutions that live in a nonlinear manifold, has emerged as the nonlinear extension of the modal analysis. One of the fundamental question is: what remains valid if we add unilateral contact conditions ? The computation of nonsmooth modes amounts to computing periodic solutions, performing the parametric continuation of solution branches and studying the stability of these branches. This calls for time integration schemes for IVP an BVP that satisfy some geometric criteria: conservation of energy, reduced numerical dispersion, symplecticity as we described before. Though the question of conservation of energy for unilateral contact has been discussed in [28], the other questions remain open. For the shooting technique and the study of stability, we need to compute the Jacobian matrix of the flow with respect to initial conditions, the so-called saltation matrix [76], [85] for nonsmooth flows. The eigenvalues of this matrix are the Floquet multipliers that give some information on the stability of the periodic solutions. The question of an efficient computation of this matrix is also an open question. For the continuation, the question is also largely open since the continuity of the solutions with respect to the parameters is not ensured.
- Extension to elastic continuum media . This is a difficult task. First of all, the question of the mathematical model for the dynamic continuum problem with unilateral contact raises some problems of well–posedness. For instance, the need for an impact law is not clear in some cases. If we perform

a semi–discretization in space with classical techniques (Finite Element Methods, Finite Difference Schemes), we obtain a discrete system for which the impact law is needed. Besides all the difficulties that we enumerate for discrete systems in the previous paragraph, the space discretization also induces numerical dispersion that may destroy the periodic solutions or renders their computation difficult. The main targeted applications for this research are cable–systems, string musical instruments, and seismic response of electrical circuit breakers with Schneider Electric.

- Computation of solutions of nonsmooth time Boundary Value Problems (BVP) (collocation, shooting) . The technique developed in the two previous items can serve as a basis for the development of more general solvers for nonsmooth BVP that can be for instance found when we solve optimal control problems by direct or indirect methods, or the computation of nonlinear waves. Two directions can be envisaged:
  - Shooting and multiple shooting techniques. In such methods, we reformulate the BVP into a sequence of IVPs that are iterated through a Newton based technique. This implies the computation of Jacobians for nonsmooth flows, the question of the continuity w.r.t to initial condition and the use of semi-smooth Newton methods.
  - Finite differences and collocations techniques. In such methods, the discretization will result into a large sparse optimization problems to solve. The open questions are as follows: a) the study of convergence, b) how to locally improve the order if the solution is locally smooth, and c) how to take benefit of spectral methods.
- Continuation techniques of solutions with respect to a parameter. Standard continuation technique requires smoothness. What types of methods can be extended in the nonsmooth case (arc-length technique, nonsmooth (semi-smooth) Newton, Asymptotical Numerical Methods (ANM))

3.3.3. Numerical optimization for discrete nonsmooth problems

Participants: V. Acary, M. Brémond, F. Pérignon, B. Brogliato, C. Prieur

- Mathematical Program with Equilibrium Constraints (MPEC) for optimal control . The discrete problem that arises in nonsmooth optimal control is generally a MPEC [92]. This problem is intrinsically nonconvex and potentially nonsmooth. Its study from a theoretical point of view has started 10 years ago but there is no consensus for its numerical solving. The goal is to work with world experts of this problem (in particular M. Ferris from Wisconsin University) to develop dedicated algorithms for solving MPEC, and provide to the optimization community challenging problems.
- Second Order Cone Complementarity Problems (SOCCP) for discrete frictional systems : After some extensive comparisons of existing solvers on a large collection of examples [36], [30], the numerical treatment of constraints redundancy by the proximal point technique and the augmented Lagrangian formulation seems to be a promising path for designing new methods. From the comparison results, it appears that the redundancy of constraints prevents the use of second order methods such as semi–smooth Newton methods or interior point methods. With P. Armand (XLIM, U. de Limoges), we propose to adapt recent advances for regularizing constraints for the quadratic problem [62] for the second-order cone complementarity problem. The other question is the improvement of the efficiency of the algorithms by using accelerated schemes for the proximal gradient method that come from large–scale machine learning and image processing problems. Learning from the experience in large–scale machine learning and image processing problems, the accelerated version of the classical gradient algorithm [83] and the proximal point algorithm [44], and many of their further extensions, could be of interest for solving discrete frictional contact problems. Following the visit of Y. Kanno (University of Tokyo) and his preliminary experience on frictionless problems, we will extend its use to frictional contact problem. When we face large-scale problems, the main available solvers is based on a Gauss–Seidel strategy that is intrinsically sequential. Accelerated first-order methods could be a good alternative to take benefit of the distributed scientific computing architectures.

3.4. Axis 3: Automatic Control

Participants: B. Brogliato, C. Prieur, V. Acary

This last axis is dedicated to the automatic control of nonsmooth dynamical systems, or the nonsmooth control of smooth systems. The first item concerns the discrete-time sliding mode control for which significant results on the implicit implementation have been obtained in the BIPOP team. The idea is to pursue this research towards state observers and differentiators (Sect 3.4.1). The second direction concerns the optimal control which brings of nonsmoothness in their solution and their formulation. After the preliminary work in BIPOP on the quadratic optimal control of Linear Complementarity systems(LCS), we propose to go further to the minimal time problem, to impacting systems and optimal control with state constraints (Sect. 3.4.2). In Sect 3.4.3 , the objective is to study the control of nonsmooth systems that contain unilateral constraint, impact and friction. The targeted systems are cable–driven systems, multi-body systems with clearances and granular materials. In Sect 3.4.4 , we will continue our work on the higher order Moreau sweeping process. Up to now, the work of BIPOP was restricted to finite-dimensional systems. In Sect 3.4.5 , we propose to extend our approach to the control of elastic structures subjected to contact unilateral constraints.

It is noteworthy that most of the problems listed below, will make strong use of the numerical tools analyzed in Axis 2, and of the Modeling analysis of Axis 1. For instance all optimal control problems yield BVPs. Control of granular materials will undoubtedly use models and numerical simulation developed in Axis 1 and 2. And so on. It has to be stressed that the type of nonsmooth models we are working with, deserve specific numerical algorithms which cannot be found in commercial software packages. One of the goals is to continue to extend our software package Siconos, and in particular the siconos/control toolbox with these developments.

3.4.1. Discrete-time Sliding-Mode Control (SMC) and State Observers (SMSO)

- *SMSO, exact differentiators:* we have introduced and obtained significant results on the implicit discretization of various classes of sliding-mode controllers [32], [34], [69], [80], [49], with successful experimental validations [70], [69], [71], [93]. Our objective is to prove that the implicit discretization can also bring advantages for sliding-mode state observers and Levant's exact differentiators, compared with the usual explicit digital implementation that generates chattering. In particular the implicit discretization guarantees Lyapunov stability and finite-time convergence properties which are absent in explicit methods.
- *High-Order SMC (HOSMC):* this family of controllers has become quite popular in the sliding-mode scientific community since its introduction by Levant in the nineties. We want here to continue the study of implicit discretization of HOSMC (twisting, super-twisting algorithms) and especially we would like to investigate the comparisons between classical (first order) SMC and HOSMC, when both are implicitly discretized, in terms of performance, accuracy, chattering suppression. Another topic of interest is stabilization in finite-time of systems with impacts and unilateral constraints, in a discrete-time setting.

3.4.2. Optimal Control

- *Linear Complementarity Systems (LCS) :* With the PhD thesis of A. Vieira, we have started to study the quadratic optimal control of LCS. Our objective is to go further with minimum-time problems. Applications of LCS are mainly in electrical circuits with set-valued components such as ideal diodes, transistors, *etc*. Such problems naturally yield MPEC when numerical solvers are sought. It is therefore intimately linked with Axis 2 objectives.
- *Impacting systems :* the optimal control of mechanical systems with unilateral constraints and impacts, largely remains an open issue. The problem can be tackled from various approaches: vibro-impact systems (no persistent contact modes) that may be transformed into discrete-time mappings *via* the impact Poincaré map; or the classical integral action minimization (Bolza problem) subjected to the complementarity Lagrangian dynamics including impacts.

- *State constraints, generalized control :* this problem differs from the previous two, since it yields Pontryagin's first order necessary conditions that take the form of an LCS with higher relative degree between the complementarity variables. This is related to the numerical techniques for the higher order sweeping process [33].

3.4.3. Control of nonsmooth discrete Lagrangian systems

- *Cable–driven systems:* these systems are typically different from the cable-car systems, and are closer in their mechanical structure to so-called tensegrity structures. The objective is to actuate a system *via* cables supposed in a first instance to be flexible (slack mode) but non-extensible in their longitudinal direction. This gives rise to complementarity conditions, one big difference with usual complementarity Lagrangian systems being that the control actions operate directly in one of the complementary variables (and not in the smooth dynamics as in cable-car systems). Therefore both the cable models and the control properties are expected to differ a lot from what we may use for cableway systems (for which guaranteeing a positive cable tension is usually not an issue, hence avoiding slack modes, but the deformation of the cables due to the nacelles and cables weights, is an important factor). Tethered systems are a close topic.
- *Multi-body systems with clearances:* our approach is to use models of clearances with dynamical impact effects, *i.e.* within Lagrangian complementarity systems. Such systems are strongly underactuated due to mechanical play at the joints. However their structure, as underactuated systems, is quite different from what has been usually considered in the Robotics and Control literature. In the recent past we have proposed a thorough numerical robustness analysis of various feedback collocated and non-collocated controllers (PD, linearization, passivity-based). We propose here to investigate specific control strategies tailored to such underactuated systems [48].
- *Granular systems:* the context is the feedback control of granular materials. To fix the ideas, one may think of a "juggling" system whose "object" (uncontrolled) part consists of a chain of aligned beads. Once the modeling step has been fixed (choice of a suitable multiple impact law), one has to determine the output to be controlled: all the beads, some of the beads, the chain's center of mass (position, velocity, vibrational magnitude and frequency), *etc*. Then we aim at investigating which type of controller may be used (output or state feedback, "classical" or sinusoidal input with feedback through the magnitude and frequency) and especially which variables may be measured/observed (positions and/or velocities of all or some of the beads, position and/or velocity of the chain's center of gravity). This topic follows previous results we obtained on the control of juggling systems [50], with increasing complexity of the "object"'s dynamics. The next step would be to extend to 2D and then 3D granular materials. Applications concern vibrators, screening, transport in mining and manufacturing processes.
- *Stability of structures:* our objective here is to study the stability of stacked blocks in 2D or 3D, and the influence on the observed behavior (numerically and/or analytically) of the contact/impact model.

3.4.4. Switching LCS and DAEs, higher-order sweeping process (HOSwP)

- We have gained a strong experience in the field of complementarity systems and distribution differential inclusions [33], [51], that may be seen as some kind of switching DAEs. We plan to go further with non-autonomous HOSwP with switching feedback inputs and non-uniform vector relative degrees. Switching linear complementarity systems can also be studied, though the exact relationships between both point of views remain unclear at the present time. This axis of research is closely related to cyber-physical systems in section 3.2 .

3.4.5. Control of Elastic (Visco-plastic) systems with contact, impact and friction

- *Stabilization, trajectory tracking:* until now we have focused on the stability and the feedback control of systems of rigid bodies. The proposal here is to study the stabilization of flexible systems (for instance, a "simple" beam) subjected to unilateral contacts with or without set-valued friction

(contacts with obstacles, or impacts with external objects line particle/beam impacts). This gives rise to varying (in time and space) boundary conditions. The best choice of a good contact law is a hard topic discussed in the literature.

- *Cableway systems (STRMTG, POMA):* cable-car systems present challenging control problems because they usually are underactuated systems, with large flexibilities and deformations. Simplified models of cables should be used (Ritz-Galerkin approach), and two main classes of systems may be considered: those with moving cable and only actuator at the station, and those with fixed cable but actuated nacelles. It is expected that they possess quite different control properties and thus deserve separate studies. The nonsmoothness arises mainly from the passage of the nacelles on the pylons, which induces frictional effects and impacts. It may certainly be considered as a nonsmooth set-valued disturbance within the overall control problem.

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 6.1.1) 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 6.3.1) 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 6.2 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 (6.2.1). 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).

BEAGLE Project-Team

3. Research Program

3.1. Introduction

As stated above, the research topics of the BEAGLE Team are centered on the modelization and simulation of cellular processes. More specifically, we focus on two specific processes that govern cell dynamics and behavior: Biophysics and Evolution. We are strongly engaged into the integration of these level of biological understanding.

3.2. Research axis 1: Computational cellular biochemistry

Biochemical kinetics developed as an extension of chemical kinetics in the early 20th century and inherited the main hypotheses underlying Van't Hoff's law of mass action : a perfectly-stirred homogeneous medium with deterministic kinetics. This classical view is however challenged by recent experimental results regarding both the movement and the metabolic fate of biomolecules. First, it is now known that the diffusive motion of many proteins in cellular media exhibits deviations from the ideal case of Brownian motion, in the form of position-dependent diffusion or anomalous diffusion, a hallmark of poorly mixing media. Second, several lines of evidence indicate that the metabolic fate of molecules in the organism not only depends on their chemical nature, but also on their spatial organisation – for example, the fate of dietary lipids depends on whether they are organized into many small or a few large droplets (see e.g. [36]). In this modern-day framework, cellular media appear as heterogeneous collections of contiguous spatial domains with different characteristics, thus providing spatial organization of the reactants. Moreover, the number of implicated reactants is often small enough that stochasticity cannot be ignored. To improve our understanding of intracellular biochemistry, we study spatiotemporal biochemical kinetics using computer simulations (particle-based spatially explicit stochastic simulations) and mathematical models (age-structured PDEs).

3.3. Research axis 2: Models for Molecular Evolution

We study the processes of genome evolution, with a focus on large-scale genomic events (rearrangements, duplications, transfers). We are interested in deciphering general laws which explain the organization of the genomes we observe today, as well as using the knowledge of these processes to reconstruct some aspects of the history of life. To do so, we construct mathematical models and apply them either in a "forward" way, *i.e.* observing the course of evolution from known ancestors and parameters, by simulation (*in silico experimental evolution*) or mathematical analysis (*theoretical biology*), or in a "backward" way, *i.e.* reconstructing ancestral states and parameters from known extant states (*phylogeny, comparative genomics*). Moreover we often mix the two approaches either by validating backwards reconstruction methods on forward simulations, or by using the forward method to test evolutionary hypotheses on biological data.

3.4. Research axis 3: Computational systems biology of neurons and astrocytes

Brain cells are rarely considered by computational systems biologists, though they are especially well suited for the field: their major signaling pathways are well characterized, the cellular properties they support are well identified (e.g. synaptic plasticity) and eventually give rise to well known functions at the organ scale (learning, memory). Moreover, electro-physiology measurements provide us with an experimental monitoring of signaling at the single cell level (sometimes at the sub-cellular scale) with unrivaled temporal resolution (milliseconds) over durations up to an hour. In this research axis, we develop modeling approaches for systems biology of both neuronal cells and glial cells, in particular astrocytes. We are mostly interested in understanding how the pathways implicated in the signaling between neurons, astrocytes and neurons-astrocytes interactions implement and regulate synaptic plasticity.

3.5. Research axis 4: Evolutionary Systems Biology

This axis, consisting in integrating the two main biological levels we study, is a long-standing and long-term objective in the team. These last years we did not make significant advances in this direction and we even removed this objective from last year's report. However the evolution of the team staff and projects allows us to give it back its central place. We now have the forces and ideas to progress. We have several short and middle term projects to integrate biochemical data and evolution. In particular we are analysing with an evolutionary perspective the 3D conformation of chromosomes, the regulatory landscape of genomes, the chromatin-associated proteins.

DRACULA Project-Team

3. Research Program

3.1. Mixed-effect models and statistical approaches

Most of biological and medical data our team has to deal with consist in time series of experimental measurements (cell counts, gene expression level, etc.). The intrinsic variability of any biological system complicates its confrontation to models. The trivial use of means, eliminating the data variance, is but a second-best solution. Furthermore, the amount of data that can be experimentally generated often limits the use of classical mathematical approaches because model's identifiability or parameter identifiability cannot be obtained. In order to overcome this issue and to efficiently take advantage of existing and available data, we plan to use mixed effect models for various applications (for instance: leukemia treatment modeling, immune response modeling). Such models were initially developed to account for individual behaviors within a population by characterizing distributions of parameter values instead of a unique parameter value. We plan to use those approaches both within that frame (for example, taking into account longitudinal studies on different patients, or different mice) but also to extend its validity in a different context: we will consider different ex vivo experiments as being "different individuals": this will allow us to make the most of the experience-to-experience variations.

Such approaches need expertise in statistics to be correctly implemented, and we will rely on the presence of Céline Vial in the team to do so. Céline Vial is an expert in applied statistics and her experience already motivated the use of better statistical methods in various research themes. The increasing use of single cell technologies in biology make such approaches necessary and it is going to be critical for the project to acquire such skills.

3.2. Development of a simulation platform

We have put some effort in developing the *SiMuScale* platform, a software coded in C++ dedicated to exploring multiscale population models, since 2014. In order to answer the challenges of multi-scale modeling it is necessary to possess an all-purpose, fast and flexible modeling tool, and *SiMuScale* is the choice we made. Since it is based on a core containing the simulator, and on plug-ins that contain the biological specifications of each cell, this software will make it easier for members of the team – and potentially other modelers – to focus on the model and to capitalize on existing models, which all share the same framework and are compatible with each other. Within the next four years, *SiMuScale* should be widely accessible and daily used in the team for multi-scale modeling. It will be developed into a real-case context, the modeling of the hematopoietic stem cell niche, in collaboration with clinicians (Eric Solary, INSERM) and physicists (Bertrand Laforge, UPMC).

3.3. Mathematical and computational modeling

Multi-scale modeling of hematopoiesis is one of the key points of the project that has started in the early stage of the Dracula team. Investigated by the team members, it took many years of close discussion with biologists to get the best understanding of the key role played by the most important molecules, hormones, kinase cascade, cell communication up to the latest knowledge. An approach that we used is based on hybrid discrete-continuous models, where cells are considered as individual objects, intracellular regulatory networks are described with ordinary differential equations, extracellular concentrations with diffusion or diffusion-convection equations (see Figure 1). These modeling tools require the expertise of all team members to get the most qualitative satisfactory model. The obtained models will be applied particularly to describe normal and pathological hematopoiesis as well as immune response.

3.4. From hybrid dynamics to continuum mechanics

Hybrid discrete-continuous methods are well adapted to describe biological cells. However, they are not appropriate for the qualitative investigation of the corresponding phenomena. Therefore, hybrid model approach should be combined with continuous 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. We will continue our studies of stability, nonlinear dynamics and pattern formation. Theoretical investigations of reaction-diffusion models will be accompanied by numerical simulations and will be applied to study cell population dynamic.

3.5. Structured partial differential equations

Hyperbolic problems are also of importance when describing cell population dynamics. They are structured transport partial differential equations, in which the structure is a characteristic of the considered population, for instance age, size, maturity, etc. In the scope of multi-scale modeling, protein concentrations as structure variables can precisely indicate the nature of cellular events cells undergo (differentiation, apoptosis), by allowing a representation of cell populations in a multi-dimensional space. Several questions are still open in the study of this problem, yet we will continue our analysis of these equations by focusing in particular on the asymptotic behavior of the system (stability, oscillations) and numerical simulations.

3.6. Delay differential equations

The use of age structure in PDE often leads to a reduction (by integration over the age variable) to delay differential equations. Delay differential equations 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. Delay differential equations offer good tools to study the behavior of the systems. Our main investigation will be the effect of perturbations of the parameters, as cell cycle duration, apoptosis, differentiation, self-renewal, etc., on the behavior of the system, in relation for instance with some pathological situations. The mathematical analysis of delay differential equations is often complicated and needs the development of new criteria to be performed.

3.7. Multi-scale modeling of the immune response

The main objective of this part is to develop models that make it possible to investigate the dynamics of the adaptive CD8 T cell immune response, and in particular to focus on the consequences of early molecular events on the cellular dynamics few days or weeks later: this would help developing predictive tools of the immune response in order to facilitate vaccine development and reduce costs. This work requires a close and intensive collaboration with immunologist partners.

We recently published a model of the CD8 T cell immune response characterizing differentiation stages, identified by biomarkers, able to predict the quantity of memory cells from early measurements ([32]). In parallel, we improved our multiscale model of the CD8 T cell immune response, by implementing a full differentiation scheme, from naïve to memory cells, based on a limited set of genes and transcription factors.

Our first task will be to infer an appropriate gene regulatory network (GRN) using single cell data analysis (generate transcriptomics data of the CD8 T cell response to diverse pathogens), the previous biomarkers we identified and associated to differentiation stages, as well as piecewise-deterministic Markov processes (Ulysse Herbach's PhD thesis, ongoing).

Our second task will be to update our multiscale model by first implementing the new differentiation scheme we identified ([32]), and second by embedding CD8 T cells with the GRN obtained in our first task (see above). This will lead to a multi-scale model incorporating description of the CD8 T cell immune response both at the molecular and the cellular levels (Simon Girel's PhD thesis, ongoing).

In order to further develop our multiscale model, we will consider an agent-based approach for the description of the cellular dynamics. Yet, such models, coupled to continuous models describing GRN dynamics, are computationally expensive, so we will focus on alternative strategies, in particular on descriptions of the cellular dynamics through both continuous and discrete models, efficiently coupled. Using discrete models for low cell numbers and continuous (partial differential equations) models for large cell numbers, with appropriate coupling strategies, can lead to faster numerical simulations, and consequently can allow performing intense parameter estimation procedures that are necessary to validate models by confronting them to experimental data, both at the molecular and cellular scales.

The final objective will be to capture CD8 T cell responses in different immunization contexts (different pathogens, tumor) and to predict cellular outcomes from molecular events.

3.8. Dynamical network inference from single-cell data

Up to now, all of our multiscale models have incorporated a dynamical molecular network that was build "by hand" after a thorough review of the literature. It would be highly valuable to infer it directly from gene expression data. However, this remains very challenging from a methodological point of view. We started exploring an original solution for such inference by using the information contained within gene expression distributions. Such distributions can be acquired through novel techniques where gene expression levels are quantified at the single cell level. We propose to view the inference problem as a fitting procedure for a mechanistic gene network model that is inherently stochastic and takes not only protein, but also mRNA levels into account. This approach led to very encouraging results [34] and we will actively pursue in that direction, especially in the light of the foreseeable explosion of single cell data.

3.9. Leukemia modeling

Imatinib and other tyrosine kinase inhibitors (TKIs) have marked a revolution in the treatment of Chronic Myelogenous Leukemia (CML). Yet, most patients are not cured, and must take their treatment for life. Deeper mechanistic understanding could improve TKI combination therapies to better control the residual leukemic cell population. In a collaboration with the Hospital Lyon Sud and the University of Maryland, we have developed mathematical models that integrate CML and an autologous immune response ([29], [30] and [31]). These studies have lent theoretical support to the idea that the immune system plays a rôle in maintaining remission over long periods. Our mathematical model predicts that upon treatment discontinuation, the immune system can control the disease and prevent a relapse. There is however a possibility for relapse via a sneak-though mechanism [29]. Research in the next four years will focus in the Phase III PETALS trial. In the PETALS trial (https://clinicaltrials.gov/ct2/show/NCT02201459), the second generation TKI Nilotinib is combined with Peg-IFN, an interferon that is thought to enhance the immune response. We plan to: 1) Adapt the model to take into account the early dynamics (first three months). 2) Use a mixed-effect approach to analyse the effect of the combination, and find population and individual parameters related to treatment efficacy and immune system response. 3) Optimise long-term treatment strategies to reduce or cease treatment and make personalised predictions based on mixed-effect parameters, to minimise the long-term probability of relapse.

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 population 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 population 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).

One important longer term goal of the above is to analyse how the behaviour and dynamics of such a network of networks might be controlled by modifying it, including by subtracting 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 solution 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. Following the evaluation of the team at the end of 2017, four main axes were identified, with the last one being the more recently added one. This axis is specifically oriented towards health in general, human or animal. The first three axes are: genomics, metabolism and post-transcriptional regulation, and (c)evolution.

Notice that the division itself is based on the biological level (genomic, metabolic/regulatory, evolutionary) or main current Life Science purpose (health) rather than on the mathematical or computational methodology involved. Any choice has its part of arbitrariness. Through the one we made, we wished to emphasise the fact that the area of application of ERABLE is important for us. *It does not mean that the mathematical and computational objectives are not equally important*, but only that those are, most often, motivated by problems coming from or associated to the general Life Science goal. Notice that such arbitrariness also means that some Life Science topics will be artificially split into two different Axes. One example of this is genomics and the two main health areas currently addressed that are intrinsically inter-related for now.

Axis 1: Genomics
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: Metabolism and post-transcriptional regulation
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 networks. This raises two main classes of problems. The first is to accurately infer such networks. 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 team has so far concentrated its efforts on two main aspects concerning such interactions: metabolism and post-transcriptional regulation by small RNAs. The more special niche we have been exploring in relation to metabolism concerns the fact that the latter may be seen as an organism's immediate window into its environment. Finely understanding how species communicate through those windows, or what impact they may have on each other through them is thus important when the ultimate goal is to be able to model communities of organisms, for understanding them and possibly, on a longer term, for control. While such communication has been explored in a number of papers, most do so at a too high level or only considered couples of interacting organisms, not larger communities. The idea of investigating consortia, and in the case of synthetic biology, of using them, has thus started being developed in the last decade only, and was motivated by the fact that such consortia may perform more complicated functions than could single populations, as well as be more robust to environmental fluctuations. Another originality of the work that the team has been doing in the last decade has also been to fully explore the combinatorial aspects of the structures used (graphs or directed hypergraphs) and of the associated algorithms. As concerns post-transcriptional regulation, the team has essentially been exploring the idea that small RNAs may have an important role in the dialog between different species.

Axis 3: (Co)Evolution
Understanding how species that live in a close relationship with others may (co)evolve requires understanding for how long symbiotic relationships are maintained or how they change through time. This may have deep implications in some cases also for understanding how to control such relationships, which may be a way of controlling the impact of symbionts on the host, or the impact of the host on the symbionts and on the environment (by acting on its symbiotic partner(s)). These relationships, also called *symbiotic associations*, have however not yet been very widely studied, at least not at a large scale.

One of the problems is getting the data, meaning the trees for hosts and symbionts but even prior to that, determining with which symbionts the present-day hosts are associated (or are "infected" by as may be the term used in some contexts) which is a big enterprise in itself. The other problem is measuring the stability of the association. This has generally been done by concomitantly studying the phylogenies of hosts and symbionts, that is by doing what is called a *cophylogeny* analysis, which itself is often realised by performing what is called a *reconciliation* of two phylogenetic trees (in theory, it could be more than two but this is a problem that has not yet been addressed by the team), one for the symbionts and one for the hosts with which the symbionts are associated. This consists in mapping one of the trees (usually, the symbiont tree) to the other. Cophylogeny inherits all the difficulties of phylogeny, among which the fact that it is not possible to check the result against the "truth" as this is now lost in the past. Cophylogeny however also brings new problems of its own which are to estimate the frequency of the different types of events that could lead to discrepant evolutionary histories, and to estimate the duration of the associations such events may create.

Axis 4: Human, animal and plant health
As indicated above, this is a recent axis in the team and concerns various applications to human and animal health. In some ways, it overlaps with the three previous axes as well as with Axis 5 on the methodological aspects, but since it gained more importance in the past few years, we decided to develop more these particular applications. Most of them started through collaborations with clinicians. Such applications are currently focused on three different topics: (i) Infectiology, (ii) Rare diseases, and (iii) Cancer.

Infectiology is the oldest one. It started by a collaboration with Arnaldo Zaha from the Federal University of Rio Grande do Sul in Brazil that focused on pathogenic bacteria living inside the respiratory tract of swines. Since our participation in the H2020 ITN MicroWine, we started interested in infections affecting plants this time, and more particularly vine plants. Rare Diseases on the other hand started by a collaboration with clinicians from the Centre de Recherche en Neurosciences of Lyon (CNRL) and is focused the Taybi-Linder Syndrome (TALS) and on abnormal splicing of U12 introns, while Cancer rests on a collaboration with the Centre Léon Bérard (CLB) and Centre de Recherche en Cancérologie of Lyon (CRCL) which is focused on Breast and Prostate carcinomas and Gynaecological carcinosarcomas.

The latter collaboration was initiated through a relationship between a member of ERABLE (Alain Viari) and Dr. Gilles Thomas who had been friends since many years. G. Thomas was one of the pioneers of Cancer Genomics in France. After his death in 2014, Alain Viari took the (part time) responsibility of his team at CLB and pursued the main projects he had started.

Within Inria and beyond, the first two applications (Infectiology and Rare Diseases) may be seen as unique because of their specific focus (resp. respiratory tract of swines / vine plants on one hand, and TALS on the other). In the first case, such uniqueness is also related to the fact that the work done involves a strong computational part but also experiments *performed within ERABLE itself*.

IBIS Project-Team

3. Research Program

3.1. Analysis of qualitative dynamics of gene regulatory networks

Participants: Hidde de Jong [Correspondent], Michel Page, Delphine Ropers.

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.

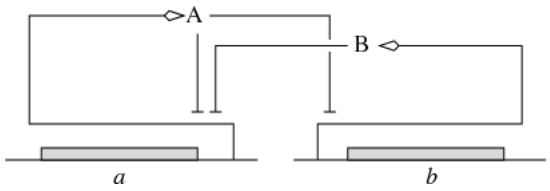
A variety of qualitative modeling formalisms have been introduced over the past decades. Boolean or logical models, which describe gene regulatory and signalling networks as discrete-time finite-state transition systems, are probably most widely used. The dynamics of these systems are governed by logical 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, Stephan Lacour, Aline Marguet, 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 of which codes 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.

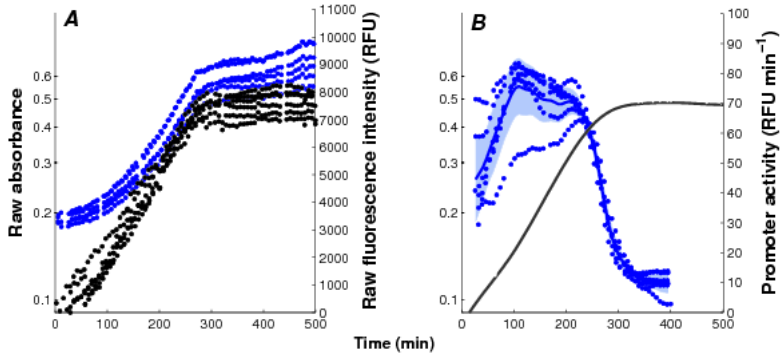


Figure 3. Monitoring of bacterial gene expression in vivo using fluorescent reporter genes (Stefan et al., PLoS Computational Biology, 11(1):e1004028, 2015). The plots show the primary data obtained in a kinetic experiment with E. coli cells, focusing on the expression of the motility gene tar in a mutant 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. 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, Marco Mauri, 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, Johannes Geiselmann [Correspondent], Hidde de Jong [Correspondent], Stephan Lacour, Marco Mauri, Tamas Muszbek, Michel Page, Antrea Pavlou, Delphine Ropers.

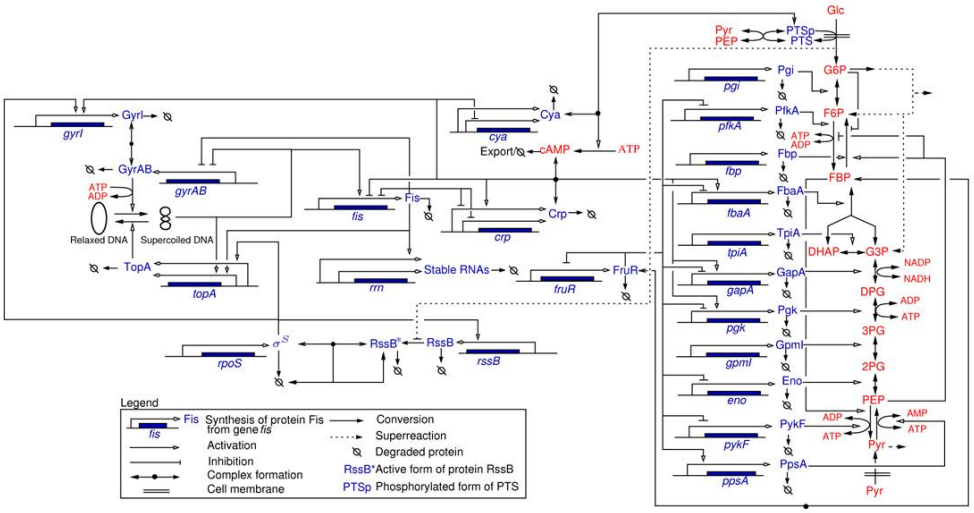


Figure 4. Network of key genes, proteins, and regulatory interactions involved in the carbon assimilation network in E. coli (Baldazzi et al., PLoS Computational Biology, 6(6):e1000812, 2010). The metabolic part includes the glycolysis/gluconeogenesis pathways as well as a simplified description of the 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 the expression of heterologous proteins in communities of interacting bacterial populations. The above projects involve collaborations with, among others, the Inria project-teams LIFEWARE (INBIO), BIOCORE, and McTAO as well as with a biophysics group at Univ Paris Descartes and a mathematical modeling group at INRA Jouy-en-Josas.

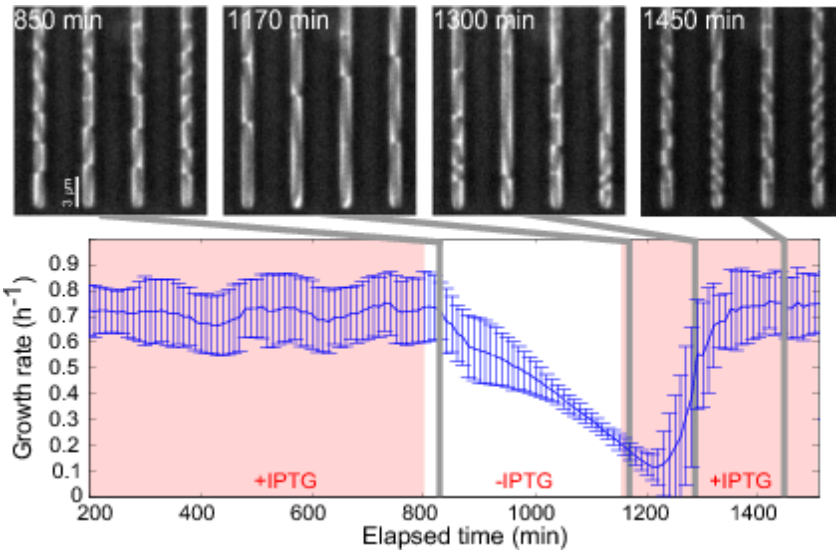


Figure 5. Growth arrest by external control of the gene expression machinery (Izard, Gomez Balderas et al., Molecular Systems Biology, 11:840, 2015). An E. coli strain in which an essential component of the gene expression machinery, the $\beta\beta'$ subunits of RNA polymerase, was put under the control 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 $\pm$ 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.

MOSAIC Team

3. Research Program

3.1. Axis1: Representation of biological organisms and their forms in silico

The modeling of organism development requires a formalization of the concept of form, *i.e.* a mathematical definition of what is a form and how it can change in time, together with the development of efficient algorithms to construct corresponding computational representations from observations, to manipulate them and associate local molecular and physical information with them. Our aim is threefold. First, we will develop new computational structures that make it possible to represent complex forms efficiently in space and time. For branching forms, the challenge will be to reduce the computational burden of the current tree-like representations that usually stems from their exponential increase in size during growth. For tissue structures, we will seek to develop models that integrate seamlessly continuous representations of the cell geometry and discrete representations of their adjacency network in dynamical and adaptive framework. Second, we will explore the use of machine learning strategies to set up robust and adaptive strategies to construct form representations in computers from imaging protocols. Finally, we will develop the notion of digital atlases of development, by mapping patterns of molecular (gene activity, hormones concentrations, cell polarity, ...) and physical (stress, mechanical properties, turgidity, ...) expressions observed at different stages of development on models representing average form development and by providing tools to manipulate and explore these digital atlases.

3.2. Axis2: Data-driven models of form development

Our aim in this second research axis will be to develop models of physiological patterning and bio-physical growth to simulate the development of 3D biological forms in a realistic way. Models of key processes participating to different aspects of morphogenesis (signaling, transport, molecular regulation, cell division, etc.) will be developed and tested *in silico* on 3D data structures reconstructed from digitized forms. The way these component-based models scale-up at more abstract levels where forms can be considered as continuums will also be investigated. Altogether, this will lead us to design first highly integrated models of form development, combining models of different processes in one computational structure representing the form, and to analyze how these processes interact in the course of development to build up the form. The simulation results will be assessed by quantitative comparison with actual form development. From a computational point of view, as branching or organ forms are often represented by large and complex data-structures, we aim to develop optimized data structures and algorithms to achieve satisfactory compromises between accuracy and efficiency.

3.3. Axis3: Plasticity and robustness of forms

In this research axis, building on the insights gained from axes 1 and 2 on the mechanisms driving form development, we aim to explore the mechanistic origin of form plasticity and robustness. At the ontogenetic scale, we will study the ability of specific developmental mechanisms to buffer, or even to exploit, biological noise during morphogenesis. For plants, we will develop models capturing morphogenetic reactions to specific environmental changes (such as water stress or pruning), and their ability to modulate or even to reallocate growth in an opportunistic manner.

At the phylogenetic scale, we will investigate new connections that can be drawn from the use of a better understanding of form development mechanisms in the evolution of forms. In animals, we will use ascidians as a model organism to investigate how the variability of certain genomes relates to the variability of their forms. In plants, models of the genetic regulation of form development will be used to test hypotheses on the evolution of regulatory gene networks of key morphogenetic mechanisms such as branching. We believe that a better mechanistic understanding of developmental processes should shed new light on old evo-devo questions related to the evolution of biological forms, such as understanding the origin of *developmental constraints*[0] how the internal rules that govern form development, such as chemical interactions and physical constraints, may channel form changes so that selection is limited in the phenotype it can achieve?

3.4. Key modeling challenges

During the project lifetime, we will address several computational challenges related to the modeling of living forms and transversal to our main research axes. During the first phase of the project, we concentrate on 4 key challenges.

3.4.1. A new paradigm for modeling tree structures in biology

There is an ubiquitous presence of tree data in biology: plant structures, tree-like organs in animals (lungs, kidney vasculature), corals, sponges, but also phylogenic trees, cell lineage trees, *etc*. To represent, analyze and simulate these data, a huge variety of algorithms have been developed. For a majority, their computational time and space complexity is proportional to the size of the trees. In dealing with massive amounts of data, like trees in a plant orchard or cell lineages in tissues containing several thousands of cells, this level of complexity is often intractable. Here, our idea is to make use of a new class of tree structures, that can be efficiently compressed and that can be used to approximate any tree, to cut-down the complexity of usual algorithms on trees.

3.4.2. Efficient computational mechanical models of growing tissues

The ability to simulate efficiently physical forces that drive form development and their consequences in biological tissues is a critical issue of the MOSAIC project. Our aim is thus to design efficient algorithms to compute mechanical stresses within data-structures representing forms as the growth simulation proceeds. The challenge consists of computing the distribution of stresses and corresponding tissue deformations throughout data-structures containing thousands of 3D cells in close to interactive time. For this we will develop new strategies to simulate mechanics based on approaches originally developed in computer graphics to simulate in real time the deformation of natural objects. In particular, we will study how meshless and isogeometric variational methods can be adapted to the simulation of a population of growing and dividing cells.

3.4.3. Realistic integrated digital models

Most of the models developed in MOSAIC correspond to specific parts of real morphogenetic systems, avoiding the overwhelming complexity of real systems. However, as these models will be developed on computational structures representing the detailed geometry of an organ or an organism, it will be possible to assemble several of these sub-models within one single model, to figure out missing components, and to test potential interactions between the model sub-components as the form develops.

Throughout the project, we will thus develop two digital models, one plant and one animal, aimed at integrating various aspects of form development in a single simulation system. The development of these digital models will be made using an agile development strategy, in which the models are created and get functional at a very early stage, and become subsequently refined progressively.

[0] Raff, R. A. (1996). The Shape of Life: Genes, Development, and the Evolution of Form. Univ. Chicago Press.

3.4.4. Development of a computational environment for the simulation of biological form development

To support and integrate the software components of the team, we aim to develop a computational environment dedicated to the interactive simulation of biological form development. This environment will be built to support the paradigm of dynamical systems with dynamical structures. In brief, the form is represented at any time by a central data-structure that contains any topological, geometric, genetic and physiological information. The computational environment will provide in a user-friendly manner tools to up-load forms, to create them, to program their development, to analyze, visualize them and interact with them in 3D+time.

NUMED Project-Team

3. Research Program

3.1. Design of complex models

3.1.1. Project team positioning

The originality of our work is the quantitative description of 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.

3.1.2. Recent results

- Population models.

  H. Leman works at the interface between mathematics and biology, thanks to probabilist and determinist studies of models of populations. More precisely, she studies and develops probabilistic models, called agent models that described the population at an individual level. Each individual is characterized by one or more phenotypic traits and by its position, which may influence at the same time its ecological behavior and its motion. From a biological point of view these models are particularly interesting since they allow to include a large variety of interactions between individuals. These processes may also be studied in details to obtain theoretical results which may be simulated thanks to exact algorithms. To get quantitative results H. Leman uses changes of scales in space and time (large population, rare mutations, long time), following various biological assumptions.

  In a first study , H. Leman tries to understand the interactions between sexual preference mechanisms and evolutive forces inside spatially structured populations. Recently she got interesting in the description of necessary conditions to facilitate the emergence of such preferences by individuals.

  As a second example, H. Leman is also interested in the modeling and study of cooperative bacterias and tries to understand the impact of spatial structures in the eco - evolutions of these bacterias. Space seems to be an essential factor to facilitate the emergence of cooperation between bacteries.
- Inviscid limit of Navier Stokes equations.

  The question of the behavior of solutions of Navier Stokes equations in a bounded domain as the viscosity goes to 0 is a classical and highly difficult open question in Fluid Mechanics. A small boundary layer, called Prandtl layer, appears near the boundary, which turns out to be unstable if the viscosity is small enough. The stability analysis of this boundary layer is highly technical and remained open since the first formal analysis in the 1940's by physicists like Orr, Sommerfeld, Tollmien, Schlichting or Lin. E. Grenier recently made a complete mathematical analysis of this spectral problem, in collaboration with T. Nguyen and Y. Guo. We rigorously proved that any shear layer is spectrally and linearly unstable if the viscosity is small enough, which is the first mathematical result in that field. We also get some preliminary nonlinear results. A book on this subject is in preparation, already accepted by Springer.
- Numerical analysis of complex fluids: the example of avalanches.

  This deals with the development of numerical schemes for viscoplastic materials (namely with Bingham or Herschell-Bulkley laws). Recently, with other colleagues, Paul Vigneaux finished the design of the first 2D well-balanced finite volume scheme for a shallow viscoplastic model. It is illustrated on the famous Taconnaz avalanche path in the Mont-Blanc, Chamonix, in the case of dense snow avalanches. The scheme deals with general Digital Elevation Model (DEM) topographies, wet/dry fronts and is designed to compute precisely the stopping state of avalanches, a crucial point of viscoplastic flows which are able to rigidify [21].

3.1.3. Collaborations

- Ecology: Orsay (C. Coron), Toulouse (IMT, M. Costa), MNHM Paris (V. Llaurens), LISC Paris (C. Smadi), ENS Paris (R. Ferrière, E. Abs), CIMAT (Mexique, J. C. P. Millan).
- Inviscid limit of Navier Stokes equations: Brown University (Y. Guo, B. Pausader), Penn State University (T. Nguyen), Orsay University (F. Rousset).
- Numerical analysis of complex fluids: Enrique D. Fernandez - Nieto (Univ. de Sevilla, Spain), Jose Maria Gallardo (Univ. de Malaga, Spain).

3.2. Parametrization of complex systems

3.2.1. Project-team positioning

Clinical data are often sparse: we have few data per patient. The number of data is of the order of the number of parameters. In this context, a natural way to parametrize complex models with real world clinical data is to use a Bayesian approach, namely to try to find the distribution of the model parameters in the population, rather than to try to identify the parameters of every single patient. This approach has been pioneered in the 90's by the Nonmem software, and has been much improved thanks to Marc Lavielle in the 2000's. Refined statistical methods, called SAEM, have been tuned and implemented in commercial softwares like Monolix.

3.2.2. Recent results

The main problem when we try to parametrize clinical data using complex systems is the computational time. One single evaluation of the model can be costly, in particular if this model involves partial differential equations, and SAEM algorithm requires hundreds of thousands of single evaluations. The time cost is then too large, in particular because SAEM may not be parallelized.

To speed up the evaluation of the complex model, we replace it by an approximate one, or so called metamodel, constructed by interpolation of a small number of its values. We therefore combine the classical SAEM algorithm with an interpolation step, leading to a strong acceleration. Interpolation can be done through a precomputation step on a fixed grid, or through a more efficient kriging step. The interpolation grid or the kriging step may be improved during SAEM algorithm in an iterative way in order to get accurate evaluations of the complex system only in the domain of interest, namely near the clinical values [14],[15].

We applied these new algorithms to synthetic data and are currently using them on glioma data. We are also currently trying to prove the convergence of the corresponding algorithms. We will develop glioma applications in the next section.

Moreover E. Ollier in his phD developed new strategies to distinguish various populations within a SAEM algorithm [23].

We have two long standing collaborations with Sanofi and Servier on parametrization issues:

- Servier: during a four years contract, we modelled the pkpd of new drugs and also study the combination and optimization of chimiotherapies.
- Sanofi: during a eight years contract, Emmanuel Grenier wrote a complete software devoted to the study of the degradation of vaccine. This software is used worldwide by Sanofi R&D teams in order to investigate the degradation of existing or new vaccines and to study their behavior when they are heated. This software has been used on flu, dengue and various other diseases.

3.2.3. Collaborations

- Academic collaborations: A. Leclerc Samson (Grenoble University)
- Medical collaborations: Dr Ducray (Centre Léon Bérard, Lyon) and Dr Sujobert (Lyon Sud Hospital)
- Industrial contracts: we used parametrization and treatment improvement techniques for Servier (four years contract, on cancer drug modeling and optimization) and Sanofi (long standing collaboration)

3.3. Multiscale models in oncology

3.3.1. Project-team positioning

Cancer modeling is the major topic of several teams in France and Europe, including Mamba, Monc and Asclepios to quote only a few Inria teams. These teams try to model metastasis, tumoral growth, vascularisation through angiogenesis, or to improve medical images quality. Their approaches are based on dynamical systems, partial differential equations, or on special imagery techniques.

Numed focuses on the link between very simple partial differential equations models, like reaction diffusion models, and clinical data.

3.3.2. Results

During 2018 we developed new collaborations with the Centre Léon Bérard (Lyon), in particular on the following topics

- Barcoding of cells: thanks to recent techniques, it is possible to mark each cell with an individual barcode, and to follow its division and descendance. The analysis of such data requires probabilistic models, in particular to model experimental bias.
- Apoptosis: the question is to investigate whether the fate of neighboring cells influence the evolution of a given cell towards apoptosis, starting from videos of in vitro drug induced apoptosis.
- Dormance: Study of the dynamics of cells under immunotherapy, starting from experimental in vitro data.
- Colorectal cancer: In vitro study of the role of stem cells in drug resistance, in colorectal cancer.

3.3.3. Collaborations

- Centre Léon Bérard (in particular: Pr Puisieux, G. Ichim, M. Plateroni, S. Ortiz).

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 [0]), 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.

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

[0] http://www.urbansim.org

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 has worked 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). 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

[0] http://www.csr.ufmg.br/dinamica/

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.

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 had been to be circumvented e.g. difficulties arising from dependencies of input variables, variables that obey a spatial organization, or switch inputs. We 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 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 work towards using sensitivity indices based on functional analysis of variance, which allow us to compare the influence of various inputs on the indicators. For example it allow the comparison of the influences of transportation and land use policies on several indicators.

AGORA Project-Team

3. Research Program

3.1. Wireless network deployment

The deployment of networks has fostered a constant research effort for decades, continuously renewed by the evolution of networking technologies. Fundamentally, the deployment problem addresses the trade off between the cost of the network to be minimized or fitted into a budget and the features and services provided by the system, that should reach a target level or be maximized. The variety of cost models and type of features gives rise to a wide scientific field. There are several cost factors of network infrastructure: components (number and capacity), energy, man power (installation and maintenance), etc. The features of the network matter as much as the metric to evaluate them. Coverage and capacity are basic features for wireless networks on which we will focus in the following. One recurrent question is therefore: What is the optimal number and position of network components to deploy so that a given territory is covered and enough networking capacity is provided?

Traditional telecommunication infrastructures were made of dedicated components, each of them providing a given set of functions. However, recently introduced paradigms yield issues on the deployment of network functions. Indeed, the last decade saw a trend towards adding more intelligence within the network. In the case of the access network, the concept of Cloud Radio Access Network (C-RAN) emerged. In the backhaul, the Evolved Packet Core (EPC) network can also benefit from virtualization techniques, as the convergence point for multiple access technologies, as imagined in the case of future 5G networks. The performance limits of a virtualized EPC remain unknown today: Is the delay introduced by this new architecture compatible with the requirements of the mobile applications? How to deploy the different network functions on generic hardware in order to maximize the quality of service?

Network component deployment. In this research direction, we address new issues of the optimal network deployment. In particular, we focus on the deployment of wireless sensor networks for environmental monitoring (e.g. atmospheric pollution). Most of current air quality monitoring systems are using conventional measuring stations, equipped with multiple lab quality sensors. These systems are however massive, inflexible and expensive. An alternative – or complementary – solution is to use low-cost flexible wireless sensor networks. One of the main challenges is to introduce adequate models for the coverage of the phenomenon. Most of the state of the art consider a generic coverage formulation based on detection ranges which are not adapted to environmental sensing. For example, pollution propagation models should take into account the inherently stochastic weather conditions. An issue is to develop adequate formulation and efficient integer linear programming (ILP) models and heuristics able to compute deployments at a relevant scale. In particular, it seems promising to adapt stochastic or robust optimization results of the operational research community in order to deals with uncertainty. Defining the quality of a coverage is also a modeling issue, which depends on the application considered. The detection of anomaly is close to a combinatorial problem. A more difficult objective is to deploy sensors in order to map the phenomenon by interpolation (or other reconstruction mechanisms). This challenge requires interdisciplinary research with fluid mechanics teams who develop numerical models of pollution propagation and practitioners like Air RhoneAlpes.

Regarding the network connectivity, another challenge is to integrate suitable wireless link models accounting for the deployment environment. For example, modeling the integration of sensors in urban areas is challenging due to the presence of neighboring walls and obstacles, as well as moving vehicles and pedestrians that may induce field scattering. Also, the urban constraints and characteristics need to be carefully modeled and considered. Indeed, the urban environment yields constraints or facilities on the deployment of sensor nodes and gateways, such as their embedding within street furniture. Understanding the structure of these spatial constraints is necessary to develop efficient optimization methods able to compute on large scale scenarios.

Network function deployment. In this research direction, we do not address network virtualization per-se, but the algorithmic and architectural challenges that virtualization brings in both radio access and core networks. As a first challenge, we focus on the evaluation of Cloud Radio Access Network solutions. The capacity of a C-RAN architecture and the way this compares to classical RAN is still an open question. The fact that C-RAN enables cooperation between the remote radio heads (RRH) served by the same base-band units (BBU) indicates an improved performance, but at the same time the resulting cells are much larger, which goes against the current trend of increasing capacity through the deployment of small cells. We propose to study the problem both from a user and a network perspective. On the user side, we use standard information theory tools, such as multiple-access channels to model C-RAN scenarios and understand their performance. On the network side, this translates in a resource allocation problem with cooperative base stations. We will extend our previous models for non-cooperative scenarios. Regarding the core network function deployment, we are interested in the specific case of Professional Mobile Radio (PMR) networks. These networks, used for public safety services and in scenarios like post-disaster relief, present the particularity of an EPC formed by a mobile wireless network. Due to its nature, the network can not be pre-planned, and the different EPC functions need to be autonomously deployed on the available network elements. We study the EPC function deployment problem as an optimization problem, constrained by the user capacity requests. User attachment mechanisms will also be proposed, adapted to the network function distribution, the global user demand, and the source/destination of the flows. These challenges are tackled as centralized optimization problems, then extended to the context of real-time decisions. Finally, in order to complete these theoretical work based on ILP models and heuristics, experiments using OpenAir Interface are used to evaluate our proposals.

3.2. Wireless data collection

With an anticipated 11-fold growth between 2014 and 2018, facing the growth of the mobile demand is the foremost challenge for mobile operators. In particular, a 100-fold increase in the number of supported connected devices, mostly newly connected objects with M2M trafic, is expected. A question therefore rises: how to cope with a dense set of M2M low bit rate traffics from energy and computing power constrained devices while classic cellular infrastructure are designed for the sparse high bit rate traffics from powerful devices?

A technological answer to the densification challenge is also embodied by long-range low-power networks such as SigFox, LoRa, NB-IoT, etc. In this context, the idea of offloading cellular traffic to different wireless access technologies is emerging as a very promising solution to relieve the traditional mobile network from its overwhelming load. In fact, offloading is already employed today, and, globally, 45% of total mobile data traffic was offloaded onto the fixed network through Wi-Fi or femtocells in 2013. Device-to-device (D2D) communications in hybrid networks, combining long-range cellular links and short-range technologies, opens even more possibilities. We aim at providing solutions that are missing for efficiently and practically mix multi-hop and cellular networks technologies.

Cellular M2M. Enabling a communication in a cellular network follows two major procedures: a resource allocation demand is first transmitted by the UE which, if successful, is followed by the actual data transmission phase, using dedicated resources allocated by the eNodeB (eNB) to the UE. This procedure was designed specifically for H2H traffic, which is bursty by nature, and it is based on the notions of session and call, activities that keep the user involved for a relatively long time and necessitate the exchange of a series of messages with the network. On the contrary, M2M traffic generates low amounts of data periodically or sporadically. Going through a signaling-heavy random access (RA) procedure to transmit one short message is strongly inefficient for both the M2M devices and the infrastructure.

In the perspective of 5G solutions, we are investigating mechanisms that regulate the M2M traffics in order to obtain good performances while keeping a reasonable quality of service (QoS) for human-to-human (H2H) terminals. The idea of piggybacking the M2M data transmission within one of the RA procedure messages is tempting and it is now considered as the best solution for this type of traffic. This means that the M2M data is transmitted on the shared resources of the RACH, and raises questions regarding the capacity of the RACH, which was not designed for these purposes. In this regard, our analysis of the access capacity of LTE-A

RACH procedure has to be adapted to multi-class scenarios, in order to understand the competition between M2M and H2H devices. Modeling based on Markov chains provides trends on system scale performances, while event-based simulations enable the analysis of the distribution of the performances over the different kinds of users. Combining both should give enough insights so as to design relevant regulation techniques and strategies. In particular two open questions that have to be tackled can be stated as: When should access resources be opened to M2M traffics without penalizing H2H performances? Does an eNodeB have a detailed enough knowledge of the system and transmit enough information to UE to regulate the traffics? The objective is to go to the analysis of achievable performances to actual protocols that take into account realistic M2M traffic patterns.

Hybrid networks. The first objective in this research axis is a realistic large-scale performance evaluation of Wi-Fi offloading solutions. While the mechanisms behind Wi-Fi offloading are now clear in the research community, their performance has only been tested in small-scale field tests, covering either small geographical areas (i.e. a few cellular base stations) and/or a small number of specific users (e.g. vehicular users). Instead, we evaluate the offloading performance at a city scale, building on real mobile network traces available in the team. First of all, through our collaboration with Orange Labs, we have access to an accurate characterization of the mobile traffic load at each base station in all major French cities. Second, a data collection application for Android devices has been developed in the team and used by hundreds of users in the Lyon metropolitan area. This application monitors and logs all the Wi-Fi access points in the coverage range of the smartphone, allowing us to build a map of Wi-Fi accessibility in some parts of the city. Combining these two data sources and completing them with simulation studies will allow an accurate evaluation of Wi-Fi offloading solutions over a large area.

On the D2D side, our focus is on the connected objects scenario, where we study the integration of short-range links and long-range technologies such as LTE, SigFox or LoRa. This requires the design of network protocols to discover and group the devices in a certain region. For this, we build on our expertise on clustering sensor and vehicular nodes. The important difference in this case is that the cellular network can assist the clustering formation process. The next step is represented by the selection of the devices that will be using the long-range links on behalf of the entire cluster. With respect to classical cluster head selection problems in ad-hoc networks, our problem distinguishes through device heterogeneity in terms of available communication technologies (not all devices have a long-range connection, or its quality is poor), energy resources (some devices might have energy harvesting capabilities) and expected lifetime. We will evaluate the proposed mechanisms both analytically (clustering problems are generally modeled by dominating set problems in graph theory) and through discrete-event simulation. Prototyping and experimental evaluation in cooperation with our industrial partners is also foreseen in this case.

3.3. Network data exploitation

Mobile devices are continuously interacting with the network infrastructure, and the associated geo-referenced events can be easily logged by the operators, for different purposes, including billing and resource management. This leads to the implicit possibility of monitoring a large percentage of the whole population with minimal cost: no other technology provides today an equivalent coverage. On the networking side, the exploration of data collected within the cellular network can be the enabler of flexible and reconfigurable cellular systems. In order to enable this vision, algorithmic solutions are needed that drive, in concert with the variations in the mobile demand, the establishment, modification, release and relocation of any type of resources in the network. This raises, in turn, the fundamental problem of understanding the mobile demand, and linking it to the resource management processes. More precisely, we contribute to answer questions about the correlation between urban areas and mobile traffic usage, in particular the spatial and temporal causalities in the usage of the mobile network.

In a different type of architecture, the one of wireless sensor networks, the spatio-temporal characteristics of the data that are transported can also be leveraged to improve on the networking performances, e.g. capacity and energy consumption. In several applications (e.g. temperature monitoring, intrusion detection), wireless sensor nodes are prone to transmit redundant or correlated information. This wastes the bandwidth

and accelerates the battery depletion. Energy and network capacity savings can be obtained by leveraging spatial and temporal correlation in packet aggregation. Packet transmissions can be reduced with an overhead induced by distributed aggregation algorithms. We aim at designing data aggregation functions that preserve data accuracy and maximize the network lifetime with low assumptions on the network topology and the application.

Mobile data analysis. In this research axis, we delve deeper in the analysis of mobile traffic. In this sense, temporal and spatial usage profiles can be built, by including in our analysis datasets providing service-level usage information. Indeed, previous studies have been generally using call detail records (CDR) or, at best, aggregated packet traffic information. This data is already very useful in many research fields, but fine-grained usage data would allow an even better understanding of the spatiotemporal characteristics of mobile traffic. To achieve this, we exploit datasets made available by Orange Labs, providing information about the network usage for several different mobile services (web, streaming, download, mail, etc.).

To obtain even richer information, we combine this operator-side data with user-side data, collected by a crowdsensing application we developed within the PrivaMov research project. While covering hundreds of thousands of users, operator data only allows to localize the user at the cell level, and only when the user is connected to the network. The crowdsensing application we are using gathers precise GPS user localization data at a high frequency. Combining these two sources of data will allow us to gain insight in possible biases introduced by operator-side data and to infer microscopic properties which, correctly modeled, can be extended to the entire user population, even those for which we do not possess crowdsensed data.

Privacy preservation is an important topic in the field of mobile data analysis. Mobile traffic data anonymization techniques are currently proposed, mainly by adding noise or removing information from the original dataset. While we do not plan to develop anonymization algorithms, we collaborate with teams working on this topic (e.g. Inria Privatics) in order to assess the impact of anonymization techniques on the spatio-temporal properties of mobile traffic data. Through a statistical analysis of both anonymized and non-anonymized data, we hope to better understand the usability of anonymized data for different applications based on the exploration of mobile traffic data.

Data aggregation. Data-aggregation takes benefit from spatial and/or temporal correlation, while preserving the data accuracy. Such correlation comes from the physical phenomenon which is observed. Temporal aggregation is mainly addressed using temporal series (e.g. ARMA) whereas spatial aggregation is now leading by compressive sensing solutions. Our objective is to get rid of the assumption of the knowledge of the network topology properties and the data traffic generated by the application, in particular for dense and massive wireless networks. Note that we focus on data-aggregation with a networking perspective, not with the background of information theory.

The rational design of an aggregation scheme implies understanding data dynamics (statistical characteristics, information representation), algorithmic optimization (aggregator location, minimizing the number of aggregators toward energy efficiency), and network dynamics (routing, medium sharing policies, node activity). We look for designing a complete aggregation chain including both intra-sensor aggregation and inter-sensor aggregation. For this, we characterize the raw data that are collected in order to understand the dynamic behind several key applications. The goal is to provide a taxonomy of the applications according to the data properties in terms of stationarity, dynamic, etc. Then, we aim to design temporal aggregation functions without knowledge of the network topology and without assumptions about the application data. Such functions should be able to self-adapt to the environment evolution. A related issue is the deployment of aggregators into the wireless network to allow spatial aggregation with respect to the energy consumption minimization, capacity saving maximization and distributed algorithm complexity. We therefore look to define dedicated protocols for each aggregation function family.

AVALON Project-Team

3. Research Program

3.1. Energy Application Profiling and Modeling

Despite recent improvements, there is still a long road to follow in order to obtain energy efficient, energy proportional and eco-responsible exascale systems by 2022. Energy efficiency is therefore a major challenge for building next generation large-scale platforms. The targeted platforms will gather hundreds of millions of 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 measurement, understanding, and analysis on how large-scale platforms consume energy. Unlike approaches [36] 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 resource 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 [39], phase detection for specific HPC applications [44], *etc.*). As a second step, we aim at designing a framework model that allows interaction, dialogue and decisions taken in cooperation among 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 time implicitly linked to “analytics” to refer to issues such as data 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. Resource-Agnostic Application Description Model

With parallel programming, users expect to obtain performance improvement, regardless its cost. For long, parallel machines have been simple enough to let a user program use them given a minimal abstraction of their hardware. For example, MPI [38] exposes the number of nodes but hides the complexity of network topology behind a set of collective operations; OpenMP [42] simplifies the management of threads on top of a shared memory machine while OpenACC [41] 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 [37]. 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 [45] 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 addressing 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 number 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 cannot 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 [43] and several issues have been raised in Clouds. Nowadays virtualization is used as the sole mechanism to allow multiple users to share resources on Clouds, but since not all components of Clouds (such as micro-architectural components) can be properly virtualized, 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.

CTRL-A Project-Team

3. Research Program

3.1. Modeling and control techniques for autonomic computing

The main objective of CTRL-A translates into a number of scientific challenges, the most important of these are:

- (i) programming language support, on the two facets of model-oriented languages, based on automata [6], and of domain specific languages, following e.g., a component-based approach [5], [1] or related to rule-based or HMI languages ;
- (ii) design methods for reconfiguration controller design in computing systems, proposing generic systems architectures and models based on transition systems [3], [8], classical continuous control or controlled stochastic systems.

  We adopt a strategy of constant experimental identification of needs and validation of proposals, in application domains like middleware platforms for Cloud systems [7], multi-core HPC architectures [11], Dynamic Partial Reconfiguration in FPGA-based hardware [2] and the IoT and smart environments [4].

Achieving the goals of CTRL-A requires multidisciplinarity and expertise from several domains. The expertise in Autonomic Computing and programming languages is covered internally by members of the Ctrl-A team. On the side of theoretical aspects of control, we have active external collaborations with researchers specialized in Control Theory, in the domain of Discrete Event Systems as well as in classical, continuous control. Additionally, an important requirement for our research to have impact is to have access to concrete, real-world computing systems requiring reconfiguration control. We target autonomic computing at different scales, in embedded systems or in cloud infrastructures, which are traditionally different domains. This is addressed by external collaborations, with experts in either hardware or software platforms, who are generally missing our competences on model-based control of reconfigurations.

DANTE Project-Team

3. Research Program

3.1. Graph-based signal processing

Participants: Paulo Gonçalves, Éric Fleury, Márton Karsai, Marion Foare, Thomas Begin.

Evolving networks can be regarded as "*out of equilibrium*" systems. Indeed, their dynamics are 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 organization 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 [76].

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 “diffusion wavelets” and “diffusion maps” pushed forward at Yale and Duke [58]. 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 for instance [71] and references therein. Other viewpoints can be found as well, including multi-resolution Markov models [79], Bayesian networks or distributed processing over sensor networks [70]. Such approaches can be particularly successful for handling static graphs and unveiling aspects of their organization 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 [59].

3.2. Theory and Structure of dynamic Networks

Participants: Christophe Crespelle, Éric Fleury, Anthony Busson, Márton Karsai, Jean-Philippe Magué, Éric Guichard, Jean-Pierre Chevrot, Tommaso Venturini.

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 [73]. 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 behaviour of complex networks [73], [63], [80], [69], to describe the observed structural and temporal heterogeneities [56], [63], [57], to detect and measure emerging community structures [60], [77], [78], to see how the functionality of networks determines their evolving structure [68], and to determine what kinds of correlations play a role in their dynamics [64], [67], [72].

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 [75]. 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 synthesising 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 [66] and its co-evolution with ongoing processes like spreading phenomena, synchronisation, evolution of consensus, random walk etc. [66], [74]. 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, Isabelle Guérin Lassous, Philippe Nain.

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 Project-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 proposed DataMove team will work 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 will address. We may also see in the coming years a convergence between HPC and Big Data, HPC platforms becoming more elastic and supporting Big

[0] Top500 Ranking, http://www.top500.org
[0] 10^{15} floating point operations per second
[0] SciDAC Review, 2010

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 will 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 will 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 will be 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 will enable 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 will make our new algorithms accessible through the team flagship software tools, **the OAR batch scheduler and the in-situ processing framework FlowVR**. We will maintain and enforce strong links with teams closely connected with large architecture design and operation (CEA DAM, BULL, Argonne National Lab), as well as scientists of other disciplines, in particular computational biologists, with whom we will elaborate and validate new usage scenarios (IBPC, CEA DAM, EDF).

3.3. Research Directions

DataMove research activity is organised around three directions. When a parallel job executes on a machine, it triggers data movements through the input data it needs to read, the results it produces (simulation results as well as traces) that need to be stored in the file system, as well as internal communications and temporary storage (for fault tolerance related data for instance). Modeling in details the simulation and the target machines to analyze scheduling policies is not feasible at large scales. We propose to investigate alternative approaches, including learning approaches, to capture and model the influence of data movements on the performance metrics of each job execution to develop **Data Aware Batch Scheduling** models and algorithms (Sec. 4.1). Experimenting new scheduling policies on real platforms at scale is unfeasible. Theoretical performance guarantees are not sufficient to ensure a new algorithm will actually perform as expected on a real platform. An intermediate evaluation level is required to probe novel scheduling policies. The second research axe focuses on the **Empirical Studies of Large Scale Platforms** (Sec. 4.2). The goal is to investigate how we could extract from actual computing centers traces information to replay the job allocations and executions on a simulated or emulated platform with new scheduling policies. Schedulers need information about jobs behavior on target machines to actually be able to make efficient allocation decisions. Asking users

[0] https://www.whitehouse.gov/the-press-office/2015/07/29/executive-order-creating-national-strategic-computing-initiative

to caracterize jobs often does not lead to reliable information. The third research direction **Integration of High Performance Computing and Data Analytics** (Sec. 4.3) addresses the data movement issue from a different perspective. New data analysis techniques on the HPC platform introduce new type of workloads, potentially more data than compute intensive, but could also enable to reduce data movements by directly enabling to pipe-line simulation execution with a live analysis of the produced results. Our goal is here to investigate how to program and schedule such analysis workflows in the HPC context.

POLARIS Project-Team

3. Research Program

3.1. Sound and Reproducible Experimental Methodology

Participants: Vincent Danjean, Nicolas Gast, Guillaume Huard, Arnaud Legrand, Patrick Loiseau, 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], [57], UIUC [75], [90], [78] and ANL [103], Inria Bordeaux [63] and Grenoble [105], ...) 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], [74] 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 [100], [50]

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. [49] 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 [61], 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 [53] and the validity of the underlying network models [51], [98]. Many simulators of MPI applications have been developed by renowned HPC groups (e.g., at SDSC [96], BSC [47], UIUC [104], Sandia Nat. Lab. [99], ORNL [60] or ETH Zürich [76] 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) [65], [58], 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 [69], 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 [59]. 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 [48]. 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 [70], [79], [102], and has been successfully applied in various domains: wireless networks [52], computer-based systems [73], [84], [97], epidemic or rumour propagation [62], [77] and bike-sharing systems [66]. It is also used to develop distributed control strategies [101], [83] or to construct approximate solutions of stochastic model checking problems [54], [55], [56].

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 [70], we would like to be able to handle heterogeneous or uncertain dynamics. Typical applications are caching mechanisms [73] or bike-sharing systems [67]. 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 [71] to build distributed control algorithms [64] and optimal pricing mechanisms [72].

3.5. Distributed Learning in Games and Online Optimization

Participants: Nicolas Gast, Bruno Gaujal, Arnaud Legrand, Patrick Loiseau, 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 [68], [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.

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 [84]. 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], [72], [73], [83], 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], [70]; 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 [85] 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 [81]. 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 [85]; (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 [80].

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, which 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 [74], [75], [79]. 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 general sparse matrix and tensor computations; and (ii) the mapping of tasks (mostly the sub-tasks of the mentioned solvers) onto modern computing platforms. We focus on the development and the 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 [69], [82], [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 [71]. 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.

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*. 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.

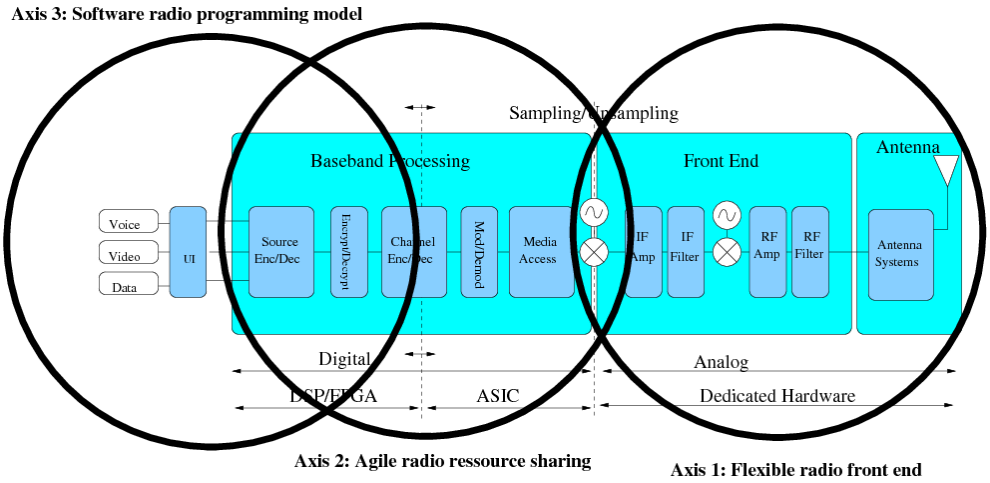


Figure 3. Center of interest for each of the three Socrate research axes with respect to a generic software radio terminal.

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, Samir Perlaza, Leonardo Sampaio Cardoso, Malcolm Egan.

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, 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. Evolution of the Socrate team

In 2018 the Socrate team has decided to split in two teams: the Maracas team will consist of the activities of Socrate Axis 2 and be directed by Jean-Marie Gorce, and the Socrate team which will consist in the Axis 1 and 3 of the current version of Socrate. This change is explicit since september 2018 as the Maracas team is created.

Chroma Project-Team

3. Research Program

3.1. Introduction

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.

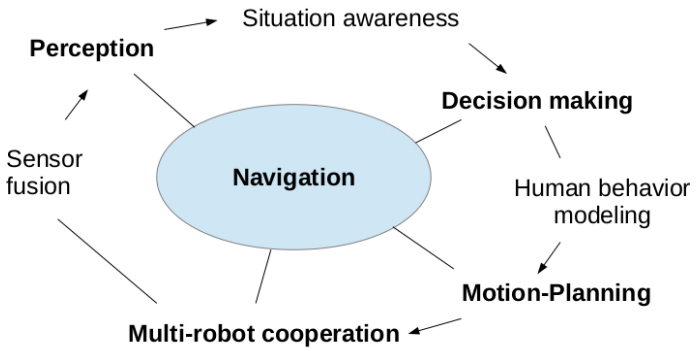


Figure 1. Research themes of the team and their relation

We present here after our approaches to address these different themes of research, and how they combine altogether to contribute to the general problem of robot navigation. Chroma pays particular attention to the problem of autonomous navigation in highly dynamic environments populated by humans and cooperation in multi-robot systems. We share this goal 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), and iCeiRA [0] laboratory in Taipei, to cite a few. Chroma collaborates 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, Christian Wolf, Ozgur Erkent, Alessandro Renzaglia, Rabbia Asghar, Jean-Alix David, Thomas Genevois, Jerome Lussereau, Anshul Paigwar, Lukas Rummelhard.

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

3.2.1. Bayesian perception

Context. Perception is known to be one of the main bottlenecks for robot motion autonomy, in particular when navigating in open and dynamic environments is subject to strong real-time and uncertainty constraints. 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 Ph.D. thesis of Christophe Coue [55] and further developed in the team [0]. The basic idea is to combine a Bayesian filter with a probabilistic grid representation of both the space and the motions. 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 (in particular the IRT Security for autonomous vehicle and Toyota 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 *CMCDOT* (Conditional Monte Carlo Dense Occupancy Tracker) framework [83] which is still under development.

This work is currently mainly performed in the scope of the "Security for Autonomous Vehicle (SAV)" project (IRT Nanoelec), and more recently in cooperation with some Industrial Companies (see section New Results for more details on the non confidential industrial cooperation projects).

Objectives. 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 (Figure 2 .a illustrates). Another 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. We also aim at developing strong partnerships with non-academic partners in order to adapt and move the technology closer to the market.

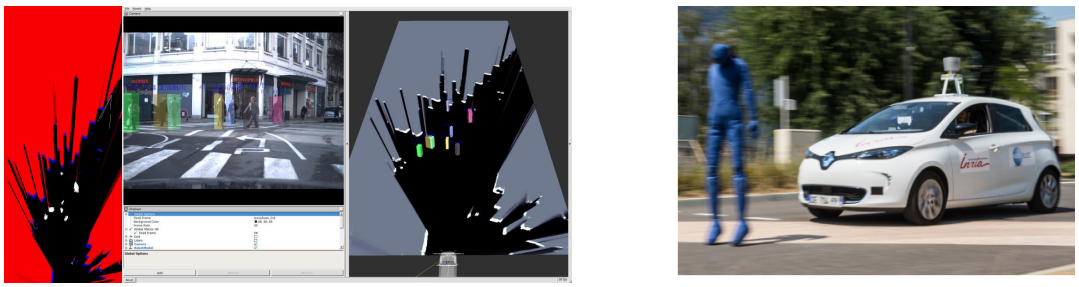


Figure 2. a. Illustration of the Bayesian Perception Paradigm: Filtered occupancy grids, enhanced with motion estimations (vectors) and object detection (colored boxes) b. Autonomous Zoe car of Inria/Chroma.

[0] The Bayesian programming formalism developed in e-Motion, pioneered (together with the contemporary work of Thrun, Burgard and Fox [91]) a systematic effort to formalize robotics problems under Probability theory–an approach that is now pervasive in Robotics.

3.2.2. System validation

Context. Testing and validating Cyber Physical Systems which are designed for operating in various real world conditions, is both an open scientific question and a necessity for a future deployment of such systems. In particular, this is the case for Embedded Perception and Decision-making Systems which are designed for future ADAS [0] and Autonomous Vehicles. Indeed, it is unrealistic to try to be exhaustive by making a huge number of experiments in various real situations. Moreover, such experiments might be dangerous, highly time consuming, and expensive. This is why we have decided to develop appropriate *realistic simulation and statistical analysis tools* for being able to perform a huge number of tests based on some previously recorded real data and on random changes of some selected parameters (the "co-simulation" concept). Such an approach might also be used in a training step of a machine learning process. This is why simulation-based validation is getting more and more popular in automotive industry and research.

This work is performed in the scope of both the SAV [0] project (IRT Nanoelec) and of the EU Enable-S3 project; it is also performed in cooperation with the Inria team Tamis in Rennes, with the objective to integrate the Tamis "Statistical Model Checking" (SMC) approach into our validation process. We are also starting to work on this topic with the Inria team Convecs, with the objective to also integrate formal methods into our validation process.

Objectives. We started to work on this new research topic in 2017. The first objective is to build a "simulated navigation framework" for: (1) constructing realistic testing environments (including the possibility of using real experiments records), (2) developing for each vehicle a simulation model including various physical and dynamic characteristics (e.g. physics, sensors and motion control), and (3) evaluating the performances of a simulation run using appropriate statistical software tools.

The second objective is to develop models and tools for automating the Simulation & Validation process, by using a selection of relevant randomized parameters for generating large database of tests and statistical results. Then, a metric based on the use of some carefully selected "Key Performance Indicator" (KPI) has to be defined for performing a statistical evaluation of the results (e.g. by using the above-mentioned SMC approach).

3.2.3. Situation Awareness and Prediction

Context. Predicting the evolution of the perceived moving agents in a dynamic and uncertain environment is mandatory for being able to safely navigate in such an environment. 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 [79]. But in human populated environments, estimating more abstract properties (e.g. object classes, affordances, agent's intentions) is also crucial to understand the future evolution of the scene. This work is carried out in the scope of the Security of Autonomous Vehicle (SAV) project (IRT Nanoelec) and of several cooperative and PhD projects with Toyota and with Renault.

Objectives. The first objective is 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 (e.g. Kalman-based, GHMM , or Gaussian Processes). In the perspective of a long-term prediction we will consider the semantic level [0] combined with planning techniques.

[0] Advance Driving Assistance System
[0] Security for Autonomous Vehicles
[0] i.e. when motion parameters are supposed to be stable during a small amount of time
[0] knowledge about agent's activities and tasks

The second objective is to build 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. Interesting published and patented results [67] have already been obtained in cooperation with Renault and UC Berkeley, by using the "Intention / Expectation" paradigm and Dynamic Bayesian Networks. 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 us to overcome the shortcomings of rules-based reasoning approaches which often show good results in low complexity situations, but which lead to a lack of scalability and of long terms predictions capabilities.

3.2.4. 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.

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 [71] (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 [73], which extends a heuristic solution derived by the team of Prof. Antonio Bicchi [51] 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 [49], [69], [61]. Recently, this sensor fusion problem has been successfully addressed by enforcing observability constraints [63], [64] and by using optimization-based approaches [68], [60], [70], [65], [78]. 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 [72] and [74]. 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.

[0] Navigation autonome des drones aériens avec la fusion des données visuelles et inertielles, lead by A. Martinelli, Chroma.

3.3. Navigation and cooperation in dynamic environments

Participants: Olivier Simonin, Anne Spalanzani, Jilles S. Dibangoye, Christian Wolf, Laetitia Matignon, Fabrice Jumel, Jacques Saraydaryan, Christian Laugier, Alessandro Renzaglia, Mohamad Hobballah, Vincent Le Doze.

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. 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

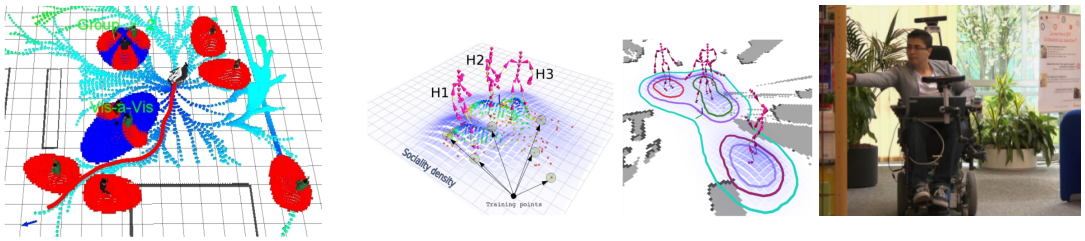


Figure 3. Illustrations of a. the Risk-RRT planning b. the human interaction space model c. experiment with the wheelchair.

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 [59], the MIT [48], the Autonomous Intelligent Systems lab in Freiburg [52], or the LAAS [80]. 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). 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 previous 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 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).

[0] Steven M. LaValle, Planning Algorithms, Cambridge University Press, 2006.
[0] known environment without uncertainty

We also investigate the problem of learning recurring human displacements - or flows of humans - from robots embedded sensors. It has been shown that such recurring behaviors can be mapped from spatial-temporal observations, as in [92]. In this context, we explore counting-based mapping models [66] to learn motion probabilities in cells of a grid representing the environment. Then we can revisit cost-function of path-planning algorithms (eg. A*) by integrating the risk to encountering humans in opposite direction. We also aim at demonstrating the efficiency of the approach with real robots evolving in dense human-populated environments.

Recently we investigated the automatic learning of robot navigation in complex environments based on specific tasks and from visual input. We address this problem by combining computer vision, machine learning (deep-learning), and robotics path planning (see 7.4.2).

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 [62], [90], [96]). 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 and the ANR Hianic.

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.

[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.
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[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.

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) [57]. 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 [93] the interest of such an approach for driverless vehicle traffic optimization.

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 explore several approaches :

- Combining MA-SDM, machine learning and RO [0] techniques to deal with global-local optimization in multi-agent/robot systems. In 2016, we started a collaboration with the VOLVO Group, in Lyon, to deal with VRP problems and optimization of goods distribution using a fleet of autonomous vehicles. We also explore such a methodology in the framework of the collaboration with the team of Prof. G. Czibula (Cluj Univiersity, Romania).
- Defining heuristics by decentralizing global exact solutions. We explore this methodology to deal with dynamic problems such as the patrolling of moving persons (see [86]). We also deal with dynamic-MRR (Multi-Robot Routing) problems in the context of the PhD of M. Popescu, see Section 7.5.1.2 .
- Online incremental refining of the environment representation. This allows us to revisit mapping/coverage techniques and problems, see section 7.5.2.1 [77].

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 continuously changing and growing (see [81]).

In Lyon, the CITI Laboratory conducts research in many aspects of telecommunication, from signal theory to distributed computation. In this context, Chroma develops cooperations with the Inria team Agora [81] (wireless communication protocols) and with Dynamid team [54] (middlleware and cloud aspects), that we wish to reinforce in the next years.

[0] Operations Research

[0] see for instance the first International Workshop on Cloud and Robotics, 2016.

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.

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.

MOEX 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.

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 may also be called an ontology. An interpretation function (I) is inductively defined over the structure of the language to a structure called the domain of interpretation (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 the expressions. A set of expressions is said consistent if it has at least one model, inconsistent otherwise. An expression (δ) is then a consequence of a set of expressions (o) if it is satisfied by all of their models (noted $o \models \delta$).

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.

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.

3.2. Data interlinking with link keys

Vast amounts of RDF data are made available on the web by various institutions providing overlapping information. To be fully exploited, different representations of the same object across various data sets, often using different ontologies, have to be identified. When different vocabularies are used for describing data, it is necessary to identify the concepts they define. This task is called ontology matching and its result is an alignment A, i.e., a set of correspondences $\langle e, r, e' \rangle$ relating entities e and e' of two different ontologies by a particular relation r (which may be equivalence, subsumption, disjointness, etc.) [3].

At the data level, data interlinking is the process of generating links identifying the same resource described in two data sets. Parallel to ontology matching, from two datasets (d and d') it generates a link set, L made of pairs of resource identifier.

We have introduced link keys [3], [1] which extend database keys in a way which is more adapted to RDF and deals with two data sets instead of a single relation. More precisely, a link key is a structure $\langle K^{eq}, K^{in}, C \rangle$ such that:

- K^{eq} and K^{in} are sets of pairs of property expressions;
- C is a pair of class expressions (or a correspondence).

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. Link keys can then be used for finding equal individuals across two data sets and generating the corresponding owl:sameAs links. Link keys take into account the non functionality of RDF data and have to deal with non literal values. In particular, they may use arbitrary properties and class expressions. This renders their discovery and use difficult.

3.3. Experimental cultural knowledge evolution

Cultural evolution applies an idealised version of the theory of evolution to culture. Cultural evolution experiments are performed through multi-agent simulation: a society of agents adapts its culture through a precisely defined protocol [15]: agents perform repeatedly and randomly a specific task, called game, and their evolution is monitored. This aims at discovering experimentally the states that agents reach and the properties of these states.

Experimental cultural evolution has been successfully and convincingly applied to the evolution of natural languages [14], [16]. Agents play *language games* and adjust their vocabulary and grammar as soon as they are not able to communicate properly, i.e., they misuse a term or they do not behave in the expected way. It showed its capacity to model various such games in a systematic framework and to provide convincing explanations of linguistic phenomena. Such experiments have shown how agents can agree on a colour coding system or a grammatical case system.

We adapt this experimental strategy to knowledge representation [2]. Agents use their, shared or private, knowledge to play games and, in case of failure, they use adaptation operators to modify this knowledge. We monitor the evolution of agent knowledge with respect to its ability to perform the game (success rate) and with respect to the properties satisfied by the resulting knowledge itself. Such properties may, for instance, be:

- Agents converge to a common knowledge representation (a convergence property).
- Agents converge towards different but compatible (logically consistent) knowledge (a logical epistemic property), or towards closer knowledge (a metric epistemic property).
- That under the threat of a changing environment, agents which have operators that preserve diverse knowledge recover faster from the changes than those which have operators that converge towards a single representation (a differential property under environment change).

Our goal is to determine which operators are suitable for achieving desired properties in the context of a particular game.

MORPHEO Project-Team

3. Research Program

3.1. Shape and Appearance Modeling

Standard acquisition platforms, including commercial solutions proposed by companies such as Microsoft, 3dMD or 4DViews, now give access to precise 3D models with geometry, e.g. meshes, and appearance information, e.g. textures. Still, state-of-the-art solutions are limited in many respects: They generally consider limited contexts and close setups with typically at most a few meter side lengths. As a result, many dynamic scenes, even a body running sequence, are still challenging situations; They also seldom exploit time redundancy; Additionally, data driven strategies are yet to be fully investigated in the field. The MORPHEO team builds on the Kinovis platform for data acquisition and has addressed these issues with, in particular, contributions on time integration, in order to increase the resolution for both for shapes and appearances, on representations, as well as on exploiting recent machine learning tools when modeling dynamic scenes. Our originality lies, for a large part, in the larger scale of the dynamic scenes we consider as well as in the time super resolution strategy we investigate. Another particularity of our research is a strong experimental foundation with the multiple camera Kinovis platforms.

3.2. Dynamic Shape Vision

Dynamic Shape Vision refers to research themes that consider the motion of dynamic shapes, with e.g. shapes in different poses, or the deformation between different shapes, with e.g. different human bodies. This includes for instance shape tracking, shape registration, all these themes being covered by MORPHEO. While progress has been made over the last decade in this domain, challenges remain, in particular due to the required essential task of shape correspondence that is still difficult to perform robustly. Strategies in this domain can be roughly classified into two categories: (i) data driven approaches that learn shape spaces and estimate shapes and their variations through space parameterizations; (ii) model based approaches that use more or less constrained prior models on shape evolutions, e.g. locally rigid structures, to recover correspondences. The MORPHEO team is substantially involved in the second category that leaves more flexibility for shapes that can be modeled, an important feature with the Kinovis platform. The team is anyway also considering the first category with faces and body under clothes modeling, classes of shapes that are more likely to evolve in spaces with reasonable dimensions. The originality of MORPHEO in this axis is to go beyond static shape poses and to consider also the dynamics of shape over several frames when modeling moving shapes, this in particular with shape tracking, animation and, more recently, with face registration.

3.3. Inside Shape Vision

Another research axis is concerned with the ability to perceive inside moving shapes. This is a more recent research theme in the MORPHEO team that has gained importance. It was originally the research associated to the Kinovis platform installed in the Grenoble Hospitals. This platform is equipped with two X-ray cameras and ten color cameras, enabling therefore simultaneous vision of inside and outside shapes. We believe this opens a new domain of investigation at the interface between computer vision and medical imaging. Interesting issues in this domain include the links between the outside surface of a shape and its inner parts, especially with the human body. These links are likely to help understanding and modeling human motions. Until now, numerous dynamic shape models, especially in the computer graphic domain, consist of a surface, typically a mesh, bound to a skeletal structure that is never observed in practice but that help anyway parameterizing human motion. Learning more accurate relationships using observations can therefore significantly impact the domain.

3.4. 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 investigate how to create new dynamic scenes using recorded events.

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 [22], [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 [8]. 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 [7]. 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 [16], [28]. 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 [17]. 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 [11].

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 [7] and audio-visual learning [9].

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 [31]. Subsequently, we proposed to combine 3D representations of shape (meshes) with photometric data [29]. 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 [30]. 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 [18], [14],[13]. 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 [11].

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 [23]. 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 [21], [20]. 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 [6]. This turned out to be a very original approach that has been followed by many other researchers in computer vision and computer graphics.

PERVASIVE Project-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.

Pervasive Interaction 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 representations of 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 Julien 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, interpersonal 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. Bibliography

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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 is carried out in the doctoral research of Nachwa Abou Bakr 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. Observing and Modelling Competence and Awareness from Eye-gaze and Emotion

Humans display awareness and emotions through a variety of non-verbal channels. It is increasingly possible to record and interpret such information with available technology. Publicly available software can be used to efficiently detect and track face orientation using web cameras. Concentration can be inferred from changes in pupil size [Kahneman 66]. Observation of Facial Action Units [Ekman 71] can be used to detect both sustained and instantaneous (micro-expressions) displays of valence and excitation. Heart rate can be measured from the Blood Volume Pulse as observed from facial skin color [Poh 11]. Body posture and gesture can be obtained from low-cost RGB sensors with depth information (RGB+D) [Shotton 13] or directly from images using detectors learned using deep learning [Ramakrishna 14]. Awareness and attention can be inferred from eye-gaze (scan path) and fixation using eye-tracking glasses as well as remote eye tracking devices [Holmqvist 11]. Such recordings can be used to reveal awareness of the current situation and to predict ability to respond effectively to opportunities and threats.

This work is supported by the ANR project CEEGE in cooperation with the department of NeuroCognition of Univ. Bielefeld. Work in this area includes the Doctoral research of Thomas Guntz to be defended in 2019.

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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.

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

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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.

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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 leaderboards, 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.

TYREX Project-Team

3. Research Program

3.1. Foundations for Data Manipulation Analysis: Logics and Type Systems

We develop methods for the static analysis of queries based on logical decision procedures. Static analysis can be used to optimize runtime performance by compile-time automated modification of the code. For example, queries can be substituted by more efficient — yet equivalent — variants. The query containment problem has been a central point of research for major query languages due to its vital role in query optimization. Query containment is defined as determining if the result of one query is included in the result of another one for any dataset. We explore techniques for deciding query containment for expressive languages for querying richly structured data such as knowledge graphs. 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 expressivity, complexity, succinctness, algorithmic techniques and effective implementations. We also investigate type systems and type-checking methods for the analysis of the manipulations of structured data.

3.2. Algebraic Foundations for Query Optimization and Code Synthesis

We consider intermediate languages based on algebraic foundations for the representation, characterization, transformations and compilation of queries. We investigate extensions of the relational algebra for optimizing expressive queries, and in particular recursive queries. We explore monads and in particular monad comprehensions and monoid calculus for the generation of efficient and scalable code on big data frameworks. When transforming and optimizing algebraic terms, we rely on cost-based searches of equivalent terms. We thus develop cost models whose purpose is to estimate the time, space and network costs of query evaluation. One difficulty is to estimate these costs in architectures where data and computations are distributed, and where the modeling of data transfers is essential.