



RESEARCH CENTER
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FIELD

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Section Scientific Foundations

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ALICE Project-Team

3. Research Program

3.1. Introduction

Computer Graphics is a quickly evolving domain of research. These last few years, both acquisition techniques (*e.g.*, range laser scanners) and computer graphics hardware (the so-called GPU's, for Graphics Processing Units) have made considerable advances. However, despite these advances, fundamental problems still remain open. For instance, a scanned mesh composed of hundred million triangles cannot be used directly in real-time visualization or complex numerical simulation. To design efficient solutions for these difficult problems, ALICE studies two fundamental issues in Computer Graphics:

- the representation of the objects, *i.e.*, their geometry and physical properties;
- the interaction between these objects and light.

Historically, these two issues have been studied by independent research communities. However, we think that they share a common theoretical basis. For instance, multi-resolution and wavelets were mathematical tools used by both communities [42]. We develop a new approach, which consists in studying the geometry and lighting from the *numerical analysis* point of view. In our approach, geometry processing and light simulation are systematically restated as a (possibly non-linear and/or constrained) functional optimization problem. This type of formulation leads to algorithms that are more efficient. Our long-term research goal is to find a formulation that permits a unified treatment of geometry and illumination over this geometry.

3.2. Geometry Processing for Engineering

Keywords: Mesh processing, parameterization, splines

Geometry processing recently emerged (in the middle of the 90's) as a promising strategy to solve the geometric modeling problems encountered when manipulating meshes composed of hundred millions of elements. Since a mesh may be considered to be a *sampling* of a surface - in other words a *signal* - the *digital signal processing* formalism was a natural theoretic background for this subdomain (see *e.g.*, [44]). Researchers of this domain then studied different aspects of this formalism applied to geometric modeling.

Although many advances have been made in the geometry processing area, important problems still remain open. Even if shape acquisition and filtering is much easier than 30 years ago, a scanned mesh composed of hundred million triangles cannot be used directly in real-time visualization or complex numerical simulation. For this reason, automatic methods to convert those large meshes into higher level representations are necessary. However, these automatic methods do not exist yet. For instance, the pioneer Henri Gouraud often mentions in his talks that the *data acquisition* problem is still open [32]. Malcolm Sabin, another pioneer of the "Computer Aided Geometric Design" and "Subdivision" approaches, mentioned during several conferences of the domain that constructing the optimum control-mesh of a subdivision surface so as to approximate a given surface is still an open problem [41]. More generally, converting a mesh model into a higher level representation, consisting of a set of equations, is a difficult problem for which no satisfying solutions have been proposed. This is one of the long-term goals of international initiatives, such as the **AIMShape** European network of excellence.

Motivated by gridding application for finite elements modeling for oil and gas exploration, in the frame of the **Gocad** project, we started studying geometry processing in the late 90's and contributed to this area at the early stages of its development. We developed the LSCM method (Least Squares Conformal Maps) in cooperation with Alias Wavefront [36]. This method has become the de-facto standard in automatic unwrapping, and was adopted by several 3D modeling packages (including Maya and Blender). We explored various applications of the method, including normal mapping, mesh completion and light simulation [2].

However, classical mesh parameterization requires to partition the considered object into a set of topological disks. For this reason, we designed a new method (Periodic Global Parameterization) that generates a continuous set of coordinates over the object [5]. We also showed the applicability of this method, by proposing the first algorithm that converts a scanned mesh into a Spline surface automatically [4].

We are still not fully satisfied with these results, since the method remains quite complicated. We think that a deeper understanding of the underlying theory is likely to lead to both efficient and simple methods. For this reason, in 2012 we studied several ways of discretizing partial differential equations on meshes, including Finite Element Modeling and Discrete Exterior Calculus. In 2013, we also explored Spectral Geometry Processing and Sampling Theory (more on this below).

3.3. Computer Graphics

Keywords: texture synthesis, shape synthesis, texture mapping, visibility

Content creation is one of the major challenges in Computer Graphics. Modeling shapes and surface appearances which are visually appealing and at the same time enforce precise design constraints is a task only accessible to highly skilled and trained designers.

In this context the team focuses on methods for by-example content creation. Given an input example and a set of constraints, we design algorithms that can automatically generate a new shape (geometry+texture). We formulate the problem of content synthesis as the joint optimization of several objectives: Preserving the local appearance of the example, enforcing global objectives (size, symmetries, mechanical properties), reaching user defined constraints (locally specified geometry, contacts). This results in a wide range of optimization problems, from statistical approaches (Markov Random fields), to combinatorial and linear optimization techniques.

As a complement to the design of techniques for automatic content creation, we also work on the representation of the content, so as to allow for its efficient manipulation. In this context we develop data-structures and algorithms targeted at massively parallel architectures, such as GPUs. These are critical to reach the interactive rates expected from a content creation technique. We also propose novel ways to store and access content defined along surfaces [6] or inside volumes [1] [35].

The team also continues research in core topics of computer graphics at the heart of realistic rendering and realistic light simulation techniques; for example, mapping textures on surfaces, or devising visibility relationships between 3D objects populating space.

BIGS Project-Team

3. Research Program

3.1. Introduction

We give here the main lines of our research that belongs to the domains of probability and statistics. For a best understanding, we made the choice to structure them in four items. Even if this choice was not arbitrary, the outlines between these items are sometimes fuzzy because each of them deals with modeling and inference and they are all interconnected.

3.2. Stochastic modeling

Our aim is to propose relevant stochastic frameworks for the modeling and the understanding of biological systems. The stochastic processes are particularly suitable for this purpose. Among them, Markov chains give a first framework for the modeling of population of cells [113], [78]. Piecewise deterministic processes are non diffusion processes also frequently used in the biological context [60], [77], [69], [63]. Among Markov model, we also developed strong expertise about processes derived from Brownian motion and Stochastic Differential Equations [103], [76], [105]. For instance, knowledge about Brownian or random walk excursions [112], [102] helps to analyse genetic sequences and to develop inference about it. However, nature provides us with many examples of systems such that the observed signal has a given Hölder regularity, which does not correspond to the one we might expect from a system driven by ordinary Brownian motion. This situation is commonly handled by noisy equations driven by Gaussian processes such as fractional Brownian motion or (in higher dimensions of the parameter) fractional fields. The basic aspects of these differential equations are now well understood, mainly thanks to the so-called *rough paths* tools [89], but also invoking the Russo-Vallois integration techniques [104]. The specific issue of Volterra equations driven by fBm, which is central for the subdiffusion within proteins problem, is addressed in [61]. Many generalizations (Gaussian or not) of this model have been recently proposed, see for instance [51] for some Gaussian locally self-similar fields, [82] for some non-Gaussian models, [54] for anisotropic models. Our team has thus contributed [59], [83], [82], [84], [97] and still contributes [53], [55], [54], [85], [73] to this theoretical study: Hölder continuity, fractal dimensions, existence and uniqueness results for differential equations, study of the laws to quote a few examples. On the other hand, because of the observation of longitudinal data for each subject in medicine, we have to care about the random effect due to the subject and to choose adapted models like mixed effect models [86], [50], [18]. In the context of health-care and cost-effectiveness analysis, we are also interested in model of aggregation of different criteria. For this purpose, we develop research about fuzzy binary measures and Choquet integral [72], [90].

3.3. Estimation and control for stochastic processes

When one desires to confront theoretical probabilistic models with real data, statistical tools and control of the dynamics are obviously crucial. As matter of course, we develop inference about stochastic processes that we use for modeling, it is the heart of some of our projects. Control of stochastic processes is also a way to optimise administration (dose, frequency) of therapy.

The monograph [81] is a good reference on the basic estimation techniques for diffusion processes. Some attention has been paid recently to the estimation of the coefficients of fractional or multifractional Brownian motion according to a set of observations. Let us quote for instance the nice surveys [48], [58]. On the other hand, the inference problem for diffusions driven by a fractional Brownian motion has been in its infancy. A good reference on the question is [111], dealing with some very particular families of equations, which do not cover the cases of interest for us. We also recently proposed least-square estimators for these kind of processes [57], [98]. Inference about PDMP is also a recent subject that we want to develop. Our team has a good expertise about inference of the rate jump and the kernel of PDMP [46], [47], [45], [33].

However, there is many directions to go further into. For instance, previous works made the assumption of a complete observation of jumps and mode, that is unrealistic in practice. We want to tackle the problem of inference of "Hidden PDMP". It could be also interesting to investigate estimation followed by optimal control for ergodic PDMP. About pharmacokinetics modeling inference, several papers have been reported for the application of system identification techniques. But two issues were ignored in these previous works: presence of timing noise and identification from longitudinal data. In [49], we have proposed a bounded-error estimation algorithm based on interval analysis to solve the parameter estimation problem while taking into consideration uncertainty on observation time instants. Statistical inference from longitudinal data based on mixed effects models [86] can be performed by the *Monolix* software (<http://www.lixoft.eu/products/monolix/product-monolix-overview/>) developed by the Monolix group chaired by Marc Lavielle and France Mentré, and supported by Inria. We used it to estimate timor growth in [50].

We consider the control of stochastic processes within the framework of Markov Decision Processes [100] and their generalization known as multi-player stochastic games [110], with a particular focus on infinite-horizon problems. In this context, we are interested in the complexity analysis of standard algorithms, as well as the proposition and analysis of numerical approximate schemes for large problems in the spirit of [52]. Regarding complexity, a central topic of research is the analysis of the Policy Iteration algorithm, which has made significant progress in the last years [116], [99], [75], [65], [109], but is still not fully understood. For large problems, we have a long experience of sensitivity analysis of approximate dynamic programming algorithms for Markov Decision Processes [107], [106], [108], [88] [13], and we currently investigate whether/how similar ideas may be adapted to multi-player stochastic games.

3.4. Algorithms and estimation for graph data

A graph data structure consists of a set of nodes, together with a set of (either unordered or ordered) pairs of these nodes called edges. This type of data is frequently used in various domains of application (in particular in biology) because they provide a mathematical representation of many concepts such as physical or biological structures and networks of relationship in a population. Some attention has recently been focused in the group on modeling and inference for graph data.

Suppose that we know the value of p variables on n subjects (in many applications, we have $n \ll p$). Inference network consists in evaluating the link between two variables knowing the others. [114] gives a very good introduction and many references about network inference and mining. Gaussian Graphical model is a convenient framework to infer network between quantitative variables: there is a edge between two variables if the partial correlation between them is non zero. So the problem is to compute the partial correlations trough the concentration matrix. Many methods are available to infer and test partial correlations in the context $n \ll p$ [114], [92], [68], [71]. However, when dealing with abundance data, because inflated zero data, data are far from gaussian assumption. Some authors work only with the binary "presence-absence" indicator via log-linear [74]. Models for inflated zero variables are not used for network inference and we want to develop them.

Among graphs, trees play a special role because they offer a good model for many biological concepts, from RNA to phylogenetic trees through plant structures. Our research deals with several aspects of tree data. In particular, we work on statistical inference for this type of data under a given stochastic model (critical Galton-Watson trees for example): in this context, the structure of the tree depends on an integer-valued distribution that we estimate from the observation of either only one tree, or a forest. We also work on lossy compression of trees via linear directed acyclic graphs. These methods make us able to compute distances between tree data faster than from the original structures and with a high accuracy. These results are valuable in the context of very large trees arising for instance in biology of plants.

3.5. Regression and machine learning

Regression models or machine learning aim at inferring statistical links between a variable of interest and covariates. It amis also at clustering subjects or variables in set homogeneous sets. In biological study, it is always important to develop adapted learning methods both in the context of "standard" data and also for very massive or online data.

A first approach for regression of quantitative variable is the non-parametric estimation of its cumulative distribution function. Many methods are available to estimate conditional quantiles and test dependencies [96], [79]. Among them we have developed nonparametric estimation through local analysis via polynomial [66], [67] and we want to study properties of this estimator in order to derive measure of risk like confidence band and test. We study also many other regression models like survival analysis, spatio temporal models with covariates. Among the multiple regression models, we want to test, thanks to simulation methods, validity of their assumptions. These kind of test are called omnibus test. An omnibus test is an overall test that examines several assumptions together, the most known omnibus test is the one for testing gaussianity (that examines both skewness and kurtosis [62]).

As it concerns the analysis point of high dimensional data, our view on the topic relies on the so-called *French data analysis school*, and more specifically on Factorial Analysis tools. In this context, stochastic approximation is an essential tool (see Lebart's paper [87]), which allows one to approximate eigenvectors in a stepwise manner. A systematic study of Principal Component and Factorial Analysis has then been led by Monnez in the series of papers [95], [93], [94], in which many aspects of convergences of online processes are analyzed thanks to the stochastic approximation techniques. BiGS aims at performing accurate classification or clustering by taking advantage of the possibility of updating the information "online" using stochastic approximation algorithms [80]. We focus on several incremental procedures for regression and data analysis like linear and logistic regressions and PCA. We also focus the biological context of high-throughput bioassays in which several hundreds or thousands of biological signals are measured for a posterior analysis. The inference of the modeling conclusions from a sample of wells to the whole population requires to account for the inter-individual variability within the modeling procedure. One solution consists in using mixed effects models but up to now no similar approach exists in the field of dynamical system identification. As a consequence, we aim at developing a new solution based on an ARX (Auto Regressive model with eXternal inputs) model structure using the EM (Expectation-Maximisation) algorithm for the estimation of the model parameters.

CAMUS Team

3. Research Program

3.1. Research Directions

The various objectives we are expecting to reach are directly related to the search of adequacy between the software and the new multicore processors evolution. They also correspond to the main research directions suggested by Hall, Padua and Pingali in [31]. Performance, correction and productivity must be the users' perceived effects. They will be the consequences of research works dealing with the following issues:

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

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

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

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

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

These different parallelizing steps are schematized on figure 1 .

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

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

3.2. Static Parallelization and Optimization

Participants: Vincent Loechner, Philippe Clauss, Éric Violard, Cédric Bastoul, Jean-François Dollinger.

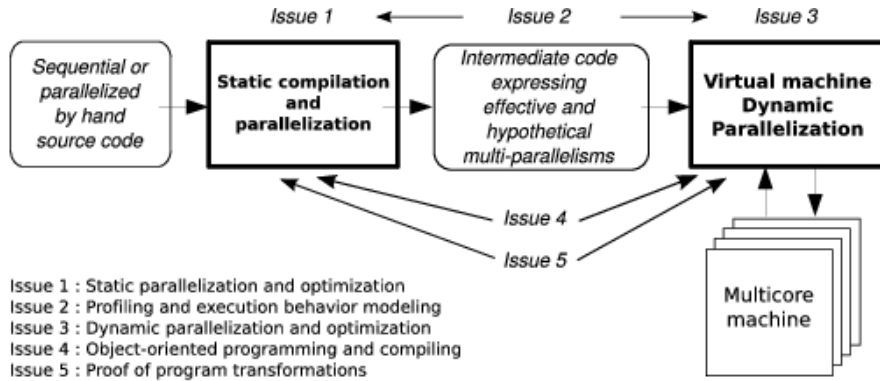


Figure 1. Automatic parallelizing steps for multicore architectures

Static optimizations, from source code at compile time, benefit from two decades of research in automatic parallelization: many works address the parallelization of loop nests accessing multi-dimensional arrays, and these works are now mature enough to generate efficient parallel code [28]. Low-level optimizations, in the assembly code generated by the compiler, have also been extensively dealt for single-core and require few adaptations to support multicore architectures. Concerning multicore specific parallelization, we propose to explore two research directions to take full advantage of these architectures: adapting parallelization to multicore architecture and expressing many potential parallelisms.

3.3. Profiling and Execution Behavior Modeling

Participants: Alain Ketterlin, Philippe Clauss, Aravind Sukumaran-Rajam, Luis Esteban Campostrini.

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

3.4. Dynamic Parallelization and Optimization, Virtual Machine

Participants: Aravind Sukumaran-Rajam, Juan Manuel Martinez Caamaño, Luis Esteban Campostrini, Artiom Baloian, Jean-François Dollinger, Mariem Saied, Daniel Salas, Philippe Clauss, Jens Gustedt, Vincent Loechner, Alain Ketterlin.

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

3.5. Proof of Program Transformations for Multicores

Participants: Éric Violard, Julien Narboux, Nicolas Magaud.

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

The optimization process can be separated into two stages: the transformations consisting in optimizing the sequential code and in exhibiting parallelism, and those consisting in optimizing the parallel code itself. The first category of optimizations can be proved within a sequential semantics. For the other optimizations, we need to work within a concurrent semantics. We expect the first stage of optimizations to produce data-race free code. For the second stage of optimizations, we will first assume that the input code is data-race free. We will prove those transformations using Appel's concurrent separation logic [32]. Proving transformations involving program which are not data-race free will constitute a longer term research goal.

CAPSID Project-Team

3. Research Program

3.1. Classifying and Mining Protein Structures and Protein Interactions

3.1.1. Context

The scientific discovery process is very often based on cycles of measurement, classification, and generalisation. It is easy to argue that this is especially true in the biological sciences. The proteins that exist today represent the molecular product of some three billion years of evolution. Therefore, comparing protein sequences and structures is important for understanding their functional and evolutionary relationships [54], [32]. There is now overwhelming evidence that all living organisms and many biological processes share a common ancestry in the tree of life. Historically, much of bioinformatics research has focused on developing mathematical and statistical algorithms to process, analyse, annotate, and compare protein and DNA sequences because such sequences represent the primary form of information in biological systems. However, there is growing evidence that structure-based methods can help to predict networks of protein-protein interactions (PPIs) with greater accuracy than those which do not use structural evidence [37], [59]. Therefore, developing techniques which can mine knowledge of protein structures and their interactions is an important way to enhance our knowledge of biology [24].

3.1.2. Quantifying Structural Similarity

Often, proteins may be divided into modular sub-units called domains, which can be associated with specific biological functions. Thus, a protein domain may be considered as the evolutionary unit of biological structure and function [58]. However, while it is well known that the 3D structures of protein domains are often more evolutionarily conserved than their one-dimensional (1D) amino acid sequences, comparing 3D structures is much more difficult than comparing 1D sequences. However, until recently, most evolutionary studies of proteins have compared and clustered 1D amino acid and nucleotide sequences rather than 3D molecular structures.

A pre-requisite for the accurate comparison of protein structures is to have a reliable method for quantifying the structural similarity between pairs of proteins. We recently developed a new protein structure alignment program called Kpax which combines an efficient dynamic programming based scoring function with a simple but novel Gaussian representation of protein backbone shape [7]. This means that we can now quantitatively compare 3D protein domains at a similar rate to throughput to conventional protein sequence comparison algorithms. We recently compared Kpax with a large number of other structure alignment programs, and we found Kpax to be the fastest and amongst the most accurate, in a CATH family recognition test [39]. The latest version of Kpax (manuscript in review) can calculate multiple flexible alignments, and thus promises to avoid such issues when comparing more distantly related protein folds and fold families.

3.1.3. Formalising and Exploiting Domain Knowledge

Concerning protein structure classification, we aim to explore novel classification paradigms to circumvent the problems encountered with existing hierarchical classifications of protein folds and domains. In particular it will be interesting to set up fuzzy clustering methods taking advantage of our previous work on gene functional classification [25], but instead using Kpax domain-domain similarity matrices. A non-trivial issue with fuzzy clustering is how to handle similarity rather than mathematical distance matrices, and how to find the optimal number of clusters, especially when using a non-Euclidean similarity measure. We will adapt the algorithms and the calculation of quality indices to the Kpax similarity measure. More fundamentally, it will be necessary to integrate this classification step in the more general process leading from data to knowledge called Knowledge Discovery in Databases (KDD) [29].

Another example where domain knowledge can be useful is during result interpretation: several sources of knowledge have to be used to explicitly characterise each cluster and to help decide its validity. Thus, it will be useful to be able to express data models, patterns, and rules in a common formalism using a defined vocabulary for concepts and relationships. Existing approaches such as the Molecular Interaction (MI) format [33] developed by the Human Genome Organization (HUGO) mostly address the experimental wet lab aspects leading to data production and curation [44]. A different point of view is represented in the Interaction Network Ontology (INO; <http://www.ino-ontology.org/> which is a community-driven ontology that is being developed to standardise and integrate data on interaction networks and to support computer-assisted reasoning [60]. However, this ontology does not integrate basic 3D concepts and structural relationships. Therefore, extending such formalisms and symbolic relationships will be beneficial, if not essential, when classifying the 3D shapes of proteins at the domain family level.

3.1.4. 3D Protein Domain Annotation and Shape Mining

A widely used collection of protein domain families is “Pfam” [28], constructed from multiple alignments of protein sequences. Integrating domain-domain similarity measures with knowledge about domain binding sites, as introduced by us in our KBDOCK approach [1], [3], can help in selecting interesting subsets of domain pairs before clustering. Thanks to our KBDOCK and Kpax projects, we already have a rich set of tools with which we can start to process and compare all known protein structures and PPIs according to their component Pfam domains. Linking this new classification to the latest “SIFTS” (Structure Integration with Function, Taxonomy and Sequence) [56] functional annotations between standard Uniprot (<http://www.uniprot.org/> sequence identifiers and protein structures from the Protein Databank (PDB) [23] could then provide a useful way to discover new structural and functional relationships which are difficult to detect in existing classification schemes such as CATH or SCOP. As part of the thesis project of Seyed Alborzi, we have made good progress in this area by developing a recommender-based data mining technique to associate enzyme classification code numbers with Pfam domains using our recently developed EC-DomainMiner program [19].

3.2. Integrative Multi-Component Assembly and Modeling

3.2.1. Context

At the molecular level, each PPI is embodied by a physical 3D protein-protein interface. Therefore, if the 3D structures of a pair of interacting proteins are known, it should in principle be possible for a docking algorithm to use this knowledge to predict the structure of the complex. However, modeling protein flexibility accurately during docking is very computationally expensive due to the very large number of internal degrees of freedom in each protein, associated with twisting motions around covalent bonds. Therefore, it is highly impractical to use detailed force-field or geometric representations in a brute-force docking search. Instead, most protein docking algorithms use fast heuristic methods to perform an initial rigid-body search in order to locate a relatively small number of candidate binding orientations, and these are then refined using a more expensive interaction potential or force-field model, which might also include flexible refinement using molecular dynamics (MD), for example.

3.2.2. Polar Fourier Docking Correlations

In our *Hex* protein docking program [48], the shape of a protein molecule is represented using polar Fourier series expansions of the form

$$\sigma(\underline{x}) = \sum_{nlm} a_{nlm} R_{nl}(r) y_{lm}(\theta, \phi), \quad (1)$$

where $\sigma(\underline{x})$ is a 3D shape-density function, a_{nlm} are the expansion coefficients, $R_{nl}(r)$ are orthonormal Gauss-Laguerre polynomials and $y_{lm}(\theta, \phi)$ are the real spherical harmonics. The electrostatic potential, $\phi(\underline{x})$, and charge density, $\rho(\underline{x})$, of a protein may be represented using similar expansions. Such representations allow the *in vacuo* electrostatic interaction energy between two proteins, A and B, to be calculated as [35]

$$E = \frac{1}{2} \int \phi_A(\underline{x})\rho_B(\underline{x})d\underline{x} + \frac{1}{2} \int \phi_B(\underline{x})\rho_A(\underline{x})d\underline{x}. \quad (2)$$

This equation demonstrates using the notion of *overlap* between 3D scalar quantities to give a physics-based scoring function. If the aim is to find the configuration that gives the most favourable interaction energy, then it is necessary to perform a six-dimensional search in the space of available rotational and translational degrees of freedom. By re-writing the polar Fourier expansions using complex spherical harmonics, we showed previously that fast Fourier transform (FFT) techniques may be used to accelerate the search in up to five of the six degrees of freedom [49]. Furthermore, we also showed that such calculations may be accelerated dramatically on modern graphics processor units [8], [6]. Consequently, we are continuing to explore new ways to exploit the polar Fourier approach.

3.2.3. Assembling Symmetrical Protein Complexes

Although protein-protein docking algorithms are improving [50], [38], it still remains challenging to produce a high resolution 3D model of a protein complex using *ab initio* techniques, mainly due to the problem of structural flexibility described above. However, with the aid of even just one simple constraint on the docking search space, the quality of docking predictions can improve dramatically [49][8]. In particular, many protein complexes involve symmetric arrangements of one or more sub-units, and the presence of symmetry may be exploited to reduce the search space considerably [22], [47], [53]. For example, using our operator notation (in which \hat{R} and \hat{T} represent 3D rotation and translation operators, respectively), we have developed an algorithm which can generate and score candidate docking orientations for monomers that assemble into cyclic (C_n) multimers using 3D integrals of the form

$$E_{AB}(y, \alpha, \beta, \gamma) = \int \left[\hat{T}(0, y, 0)\hat{R}(\alpha, \beta, \gamma)\phi_A(\underline{x}) \right] \times \left[\hat{R}(0, 0, \omega_n)\hat{T}(0, y, 0)\hat{R}(\alpha, \beta, \gamma)\rho_B(\underline{x}) \right] d\underline{x}, \quad (3)$$

where the identical monomers A and B are initially placed at the origin, and $\omega_n = 2\pi/n$ is the rotation about the principal n -fold symmetry axis. This example shows that complexes with cyclic symmetry have just 4 rigid body DOFs, compared to $6(n-1)$ DOFs for non-symmetrical n -mers. We have generalised these ideas in order to model protein complexes that crystallise into any of the naturally occurring point group symmetries (C_n, D_n, T, O, I). Although we currently use shape-based FFT correlations, the symmetry operator technique may equally be used to refine candidate solutions using a more accurate CG force-field scoring function.

3.2.4. Coarse-Grained Models

Many approaches have been proposed in the literature to take into account protein flexibility during docking. The most thorough methods rely on expensive atomistic simulations using MD. However, much of a MD trajectory is unlikely to be relevant to a docking encounter unless it is constrained to explore a putative protein-protein interface. Consequently, MD is normally only used to refine a small number of candidate rigid body docking poses. A much faster, but more approximate method is to use coarse-grained (CG) normal mode analysis (NMA) techniques to reduce the number of flexible degrees of freedom to just one or a handful of the most significant vibrational modes [43], [26], [40], [41]. In our experience, docking ensembles of NMA conformations does not give much improvement over basic FFT-based soft docking [9], and it is very computationally expensive to use side-chain repacking to refine candidate soft docking poses [2].

In the last few years, CG *force-field* models have become increasingly popular in the MD community because they allow very large biomolecular systems to be simulated using conventional MD programs [21]. Typically, a CG force-field representation replaces the atoms in each amino acid with from 2 to 4 “pseudo-atoms”, and it assigns each pseudo-atom a small number of parameters to represent its chemo-physical properties. By directly attacking the quadratic nature of pair-wise energy functions, coarse-graining can speed up MD simulations by up to three orders of magnitude. Nonetheless, such CG models can still produce useful models of very large multi-component assemblies [52]. Furthermore, this kind of coarse-graining effectively integrates out many of the internal DOFs to leave a smoother but still physically realistic energy surface [34]. We are therefore developing a “coarse-grained” scoring function for fast protein-protein docking and multi-component assembly.

3.2.5. Assembling Multi-Component Complexes and Integrative Structure Modeling

We also want to develop related approaches for integrative structure modeling using cryo-electron microscopy (cryo-EM). Thanks to recently developments in cryo-EM instruments and technologies, it is now feasible to capture low resolution images of very large macromolecular machines. However, while such developments offer the intriguing prospect of being able to trap biological systems in unprecedented levels of detail, there will also come an increasing need to analyse, annotate, and interpret the enormous volumes of data that will soon flow from the latest instruments. In particular, a new challenge that is emerging is how to fit previously solved high resolution protein structures into low resolution cryo-EM density maps. However, the problem here is that large molecular machines will have multiple sub-components, some of which will be unknown, and many of which will fit each part of the map almost equally well. Thus, the general problem of building high resolution 3D models from cryo-EM data is like building a complex 3D jigsaw puzzle in which several pieces may be unknown or missing, and none of which will fit perfectly. Although we do not have precise roadmap to a solution for the multi-component assembly problem, we wish to proceed firstly by putting more emphasis on the single-body terms in the scoring function, and secondly by using fast CG representations and knowledge-based distance restraints to prune large regions of the search space.

CAMEL Project-Team

3. Research Program

3.1. Cryptography, Arithmetic: Hardware and Software

One of the main topics for our project is public-key cryptography. After 20 years of hegemony, the classical public-key algorithms (whose security is based on integer factorization or discrete logarithm in finite fields) are currently being overtaken by elliptic curves. The fundamental reason for this is that the best algorithms known for factoring integers or for computing discrete logarithms in finite fields have — at best — a subexponential complexity, whereas the best attack known for elliptic-curve discrete logarithms has exponential complexity. As a consequence, for a given security level 2^n , the key sizes must grow linearly with n for elliptic curves, whereas they grow like n^3 for RSA-like systems. As a consequence, several governmental agencies, like the NSA (National Security Agency, USA) or the BSI (Bundesamt für Sicherheit in der Informationstechnik, Germany), now recommend to use elliptic-curve cryptosystems for new products that are not bound to RSA for backward compatibility.

Besides RSA and elliptic curves, there are several alternatives currently under study. There is a recent trend to promote alternate solutions that do not rely on number theory, with the objective of building systems that would resist a quantum computer (in contrast, integer factorization and discrete logarithms in finite fields and elliptic curves have a polynomial-time quantum solution). Among them, we find systems based on hard problems in lattices (NTRU is the most famous), those based on coding theory (McEliece system and improved versions), and those based on the difficulty to solve multivariate polynomial equations (UOV, for instance). None of them has yet reached the same level of popularity as RSA or elliptic curves for various reasons, including the presence of unsatisfactory features (like a huge public key), or the non-maturity (system still alternating between being fixed one day and broken the next day).

Returning to number theory, an alternative to RSA and elliptic curves is to use other curves and in particular genus-2 curves. These so-called hyperelliptic cryptosystems have been proposed in 1989 [28], soon after the elliptic ones, but their deployment is by far more difficult. The first problem was the group law. For elliptic curves, the elements of the group are just the points of the curve. In a hyperelliptic cryptosystem, the elements of the group are points on a 2-dimensional variety associated to the genus-2 curve, called the Jacobian variety. Although there exist polynomial-time methods to represent and compute with them, it took some time before getting a group law that could compete with the elliptic one in terms of speed. Another question that is still not yet fully answered is the computation of the group order, which is important for assessing the security of the associated cryptosystem. This amounts to counting the points of the curve that are defined over the base field or over an extension, and therefore this general question is called point-counting. In the past ten years there have been major improvements on the topic, but there are still cases for which no practical solution is known.

Another recent discovery in public-key cryptography is the fact that having an efficient bilinear map that is hard to invert (in a sense that can be made precise) can lead to powerful cryptographic primitives. The only examples we know of such bilinear maps are associated with algebraic curves, and in particular elliptic curves: this is the so-called Weil pairing (or its variant, the Tate pairing). Initially considered as a threat for elliptic-curve cryptography, they have proven to be quite useful from a constructive point of view, and since the beginning of the decade, hundreds of articles have been published, proposing efficient protocols based on pairings. A long-lasting open question, namely the construction of a practical identity-based encryption scheme, has been solved this way. The first standardization of pairing-based cryptography has recently occurred (see ISO/IEC 14888-3 or IEEE P1363.3), but the recent progress in discrete logarithms in finite fields will probably slow down its large deployment.

Despite the rise of elliptic curve cryptography and the variety of more or less mature alternatives, classical systems (based on factoring or discrete logarithm in finite fields) are still going to be widely used in the next decade, at least, due to resilience: it takes a long time to adopt new standards, and then an even longer time to renew all the software and hardware that is widely deployed.

This context of public-key cryptography motivates us to work on integer factorization, for which we have acquired expertise, both in factoring moderate-sized numbers, using the ECM (Elliptic Curve Method) algorithm, and in factoring large RSA-like numbers, using the number field sieve algorithm. The goal is to follow the transition from RSA to other systems and continuously assess its security to adjust key sizes. We also work on the discrete-logarithm problem in finite fields. This second task is not only necessary for assessing the security of classical public-key algorithms, but is also crucial for the security of pairing-based cryptography.

Another general application for the project is computer algebra systems (CAS), that rely in many places on efficient arithmetic. Nowadays, the objective of a CAS is not only to support an increasing number of features that the user might wish, but also to compute the results fast enough, since in many cases, the CAS are used interactively, and a human is waiting for the computation to complete. To tackle this question, more and more CAS use external libraries, that have been written with speed and reliability as first concern. For instance, most of today's CAS use the GMP library for their computations with big integers. Many of them will also use some external Basic Linear Algebra Subprograms (BLAS) implementation for their needs in numerical linear algebra.

During a typical CAS session, the libraries are called with objects whose sizes vary a lot; therefore being fast on all sizes is important. This encompasses small-sized data, like elements of the finite fields used in cryptographic applications, and larger structures, for which asymptotically fast algorithms are to be used. For instance, the user might want to study an elliptic curve over the rationals, and as a consequence, check its behaviour when reduced modulo many small primes; and then [s]he can search for large torsion points over an extension field, which will involve computing with high-degree polynomials with large integer coefficients.

Writing efficient software for arithmetic as it is used typically in CAS requires the knowledge of many algorithms with their range of applicability, good programming skills in order to spend time only where it should be spent, and finally good knowledge of the target hardware. Indeed, it makes little sense to disregard the specifics of the intended hardware platforms, even more so since in the past years, we have seen a paradigm shift in terms of available hardware: so far, it used to be reasonable to consider that an end-user running a CAS would have access to a single-CPU processor. Nowadays, even a basic laptop computer has a multi-core processor and a powerful graphics card, and a workstation with a reconfigurable coprocessor is no longer science-fiction.

In this context, one of our goals is to investigate and take advantage of these influences and interactions between various available computing resources in order to design better algorithms for basic arithmetic objects. Of course, this is not disconnected from the other goals, since they all rely more or less on integer or polynomial arithmetic.

CARTE Project-Team

3. Research Program

3.1. Computer Virology

From a historical point of view, the first official virus appeared in 1983 on Vax-PDP 11. At the same time, a series of papers was published which always remains a reference in computer virology: Thompson [76], Cohen [46] and Adleman [35]. The literature which explains and discusses practical issues is quite extensive [51], [53]. However, there are only a few theoretical/scientific studies, which attempt to give a model of computer viruses.

A virus is essentially a self-replicating program inside an adversary environment. Self-replication has a solid background based on works on fixed point in λ -calculus and on studies of von Neumann [80]. More precisely we establish in [42] that Kleene's second recursion theorem [65] is the cornerstone from which viruses and infection scenarios can be defined and classified. The bottom line of a virus behavior is

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

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

3.2. Computation over continuous structures

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

While the notion of a computable function over discrete data is captured by the model of Turing machines, the situation is more delicate when the data are continuous, and several non-equivalent models exist. In this case, let us mention computable analysis, which relates computability to topology [50], [79]; the Blum-Shub-Smale model (BSS), where the real numbers are treated as elementary entities [41]; the General Purpose Analog Computer (GPAC) introduced by Shannon [74] with continuous time.

3.3. Rewriting

The rewriting paradigm is now widely used for specifying, modelizing, programming and proving. It allows one to easily express deduction systems in a declarative way, and to express complex relations on infinite sets of states in a finite way, provided they are countable. Programming languages and environments with a rewriting based semantics have been developed ; see ASF+SDF [43], MAUDE [45], and TOM [71].

For basic rewriting, many techniques have been developed to prove properties of rewrite systems like confluence, completeness, consistency or various notions of termination. Proof methods have also been proposed for extensions of rewriting such as equational extensions, consisting of rewriting modulo a set of axioms, conditional extensions where rules are applied under certain conditions only, typed extensions, where rules are applied only if there is a type correspondence between the rule and the term to be rewritten, and constrained extensions, where rules are enriched by formulas to be satisfied [37], [49], [75].

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

Another interesting aspect is that it allows characteristics or properties of the modeled systems to be expressed as equational theorems, often automatically provable using the rewriting mechanism itself or induction techniques based on completion [48]. Note that the rewriting and the completion mechanisms also enable transformation and simplification of formal systems or programs.

Applications of rewriting-based proofs to computer security are various. Approaches using rule-based specifications have recently been proposed for detection of computer viruses [77], [78]. For several years, in our team, we have also been working in this direction. We already proposed an approach using rewriting techniques to abstract program behaviors for detecting suspicious or malicious programs [38], [39].

CASSIS Project-Team

3. Research Program

3.1. Introduction

Our main goal is to design techniques and to develop tools for the verification of (safety-critical) systems, such as programs or protocols. To this end, we develop a combination of techniques based on automated deduction for program verification, constraint resolution for test generation, and reachability analysis for the verification of infinite-state systems.

3.2. Automated Deduction

The main goal is to prove the validity of assertions obtained from program analysis. To this end, we develop techniques and automated deduction systems based on rewriting and constraint solving. The verification of recursive data structures relies on inductive reasoning or the manipulation of equations and it also exploits some form of reasoning modulo properties of selected operators (such as associativity and/or commutativity).

Rewriting, which allows us to simplify expressions and formulae, is a key ingredient for the effectiveness of many state-of-the-art automated reasoning systems. Furthermore, a well-founded rewriting relation can also be exploited to implement reasoning by induction. This observation forms the basis of our approach to inductive reasoning, with high degree of automation and the possibility to refute false conjectures.

The constraints are the key ingredient to postpone the activity of solving complex symbolic problems until it is really necessary. They also allow us to increase the expressivity of the specification language and to refine theorem-proving strategies. As an example of this, the handling of constraints for unification problems or for the orientation of equalities in the presence of interpreted operators (e.g., commutativity and/or associativity function symbols) will possibly yield shorter automated proofs.

Finally, decision procedures are being considered as a key ingredient for the successful application of automated reasoning systems to verification problems. A decision procedure is an algorithm capable of efficiently deciding whether formulae from certain theories (such as Presburger arithmetic, lists, arrays, and their combination) are valid or not. We develop techniques to build and to combine decision procedures for the domains which are relevant to verification problems. We also perform experimental evaluation of the proposed techniques by combining propositional reasoning (implemented by means of Boolean solvers, e.g., SAT solvers) and decision procedures to get solvers for the problem of Satisfiability Modulo Theories (SMT).

3.3. Synthesizing and Solving Constraints

Applying constraint logic programming technology in the validation and verification area is currently an active way of research. It usually requires the design of specific solvers to deal with the description language's vocabulary. For instance, we are interested in applying a solver for set constraints to evaluate set-oriented formal specifications. By evaluation, we mean the encoding of the formal model into a constraint system, and the ability for the solver to verify the invariant on the current constraint graph, to propagate preconditions or guards, and to apply a substitution calculus on this graph. The constraint solver is used for animating specifications and automatically generating abstract test cases.

3.4. Rewriting-based Safety Checking

Invariant checking and strengthening is the dual of reachability analysis, and can thus be used for verifying safety properties of infinite-state systems. In fact, many infinite-state systems are just parameterized systems which become finite state systems when parameters are instantiated. Then, the challenge is to automatically discharge the maximal number of proof obligations coming from the decomposition of the invariance conditions. For parameterized systems, we are interested in a deductive approach where states are defined by first-order formulae with equality, and proof obligations are checked by SMT solvers.

COAST Project-Team

3. Research Program

3.1. Introduction

Our scientific foundations are grounded on distributed collaborative systems supported by sophisticated data sharing mechanisms and on service oriented computing with an emphasis on orchestration and on non functional properties.

Distributed collaborative systems enable distributed group work supported by computer technologies. Designing such systems require an expertise in Distributed Systems and in Computer-supported collaborative activities research area. Besides theoretical and technical aspects of distributed systems, the design of distributed collaborative systems must take into account the human factor to offer solutions suitable for users and groups. The COAST team vision is to move away from a centralized authority based collaboration towards a decentralized collaboration where users have full control over their data that they can store locally and decide with whom to share them. The Coast team investigates the issues related to the management of distributed shared data and coordination between users and groups.

Service oriented Computing [22] is an established domain on which the ECOO, SCORE and now the Coast team have been contributing for a long time. It refers to the general discipline that studies the development of computer applications on the web. A service is an independent software program with a specific functional context and capabilities published as a service contract (or more traditionally an API). A service composition aggregates a set of services and coordinates their interactions. The scale, the autonomy of services, the heterogeneity and some design principles underlying Service Oriented Computing open new research questions that are at the basis of our research. They span the disciplines of distributed computing, software engineering and computer supported collaborative work (CSCW). Our approach to contribute to the general vision of Service Oriented Computing and more generally to the emerging discipline of Service Science has been and is still to focus on the issue of the efficient and flexible construction of reliable and secure high level services through the coordination/orchestration/composition of other services provided by distributed organizations or people.

3.2. Consistency Models for Distributed Collaborative Systems

Collaborative systems are distributed systems that allow users to share data. One important issue is to manage consistency of shared data according to concurrent access. Traditional consistency criteria such as locking, serializability, linearizability are not adequate for collaborative systems.

Causality, Convergence and Intention preservation (CCI) [25] are more suitable for developing middleware for collaborative applications.

We develop algorithms for ensuring CCI properties on collaborative distributed systems. Constraints on the algorithms are different according to the kind of distributed system and to the data structure. The distributed system can be centralized, decentralized or peer-to-peer. The type of data can include strings, growable arrays, ordered trees, semantic graphs and multimedia data.

3.3. Optimistic Replication

Replication of data among different nodes of a network allows improving reliability, fault-tolerance, and availability. When data are mutable, consistency among the different replicas must be ensured. Pessimistic replication is based on the principle of single-copy consistency while optimistic replication allows the replicas to diverge during a short time period. The consistency model for optimistic replication [24] is called eventual consistency, meaning that replicas are guaranteed to converge to the same value when the system is idle.

Our research focuses on the two most promising families of optimistic replication algorithms for ensuring CCI:

- the operational transformation (OT) algorithms [20]
- the algorithms based on commutative replicated data types (CRDT) [23].

Operational transformation algorithms are based on the application of a transformation function when a remote modification is integrated into the local document. Integration algorithms are generic, being parametrized by operational transformation functions which depend on replicated document types. The advantage of these algorithms is their genericity. These algorithms can be applied to any data type and they can merge heterogeneous data in a uniform manner.

Commutative replicated data types is a new class of algorithms initiated by WOOT [21] a first algorithm designed Without Operational Transformations. They ensure consistency of highly dynamic content on peer-to-peer networks. Unlike traditional optimistic replication algorithms, they can ensure consistency without concurrency control. CRDT algorithms rely on natively commutative operations defined on abstract data types such as lists or ordered trees. Thus, they do not require a merge algorithm or an integration procedure.

3.4. Process Orchestration and Management

Process Orchestration and Management is considered as a core discipline behind Service Management and Computing. It includes the analysis, the modelling, the execution, the monitoring and the continuous improvement of enterprise processes and is for us a central domain of studies.

Much efforts have been devoted in the past years to establish standard business process models founded on well grounded theories (e.g. Petri Nets) that meet the needs of both business analysts but also of software engineers and software integrators. This has led to heated debate in the BPM community as both points of view are very difficult to reconcile. On one side, the business people in general require models that are easy to use and understand and that can be quickly adapted to exceptional situations. On the other side, IT people need models with an operational semantic in order to be able transform them into executable artefacts. Part of our work has been an attempt to reconcile these point of views. It resulted in the development of Bonita product and more recently on our work in crisis management where the same people are designing, executing and monitoring the process as it executes. But more generally, and at a larger scale, we have been considering the problem of process spanning the barriers of organisations and thus more general problem of service composition as a way to coordinate inter organisational construction of applications providing value based on the composition of lower level services [19].

3.5. Service Composition

We are considering processes as pieces of software whose execution traverse the boundaries of organisations. This is especially true with service oriented computing where processes compose services produced by many organisations. We tackle this problem from very different perspectives, trying to find the best compromise between the need for privacy of internal processes from organisations and the necessity to publicize large part of them, proposing to distribute the execution and the orchestration of processes among the organisations themselves, and attempting to ensure non functional properties in this distributed setting [18].

Non functional aspects of service composition relate to all the properties and service agreements that one want to ensure and that are orthogonal to the actual business but that are important when a service is selected and integrated in a composition. This includes transactional context, security, privacy, and quality of service in general. Defining and orchestrating services on a large scale while providing the stakeholders with some strong guarantees on their execution is a first class problem for us. For a long time, we have proposed models and solutions to ensure that some properties (e.g. transactional properties) were guaranteed on process execution, either through design or through the definition of some protocols. Our work has also been extended to the problems of security, privacy and service level agreement among partners. These questions are still central in our work. Then, one major problem of current approaches is to monitor the execution of the compositions, integrating the distributed dimension. This problem can be tackled using event-based

algorithms and techniques. Using our event oriented composition framework DISC, we have obtained new results dedicated to the runtime verification of violations in service choreographies.

LARSEN Team

3. Research Program

3.1. Lifelong Autonomy

3.1.1. Scientific Context

So far, only a few autonomous robots have been deployed for a long time (weeks, months, or years) outside of factories or laboratories. They are mostly mobile robots that simply “move around” (e.g., vacuum cleaners or museum “guides”) and data collecting robots (e.g., boats or underwater “gliders” that collect data about the water of ocean).

A large part of the long-term autonomy community is focused on simultaneous localization and mapping (SLAM), with a recent emphasis on changing and outdoor environments [33], [48]. A more recent theme is life-long learning: during long-term deployment, we cannot hope to equip robots with everything they need to know, therefore some things will have to be learned along the way. Most of the work on this topic leverages machine learning and/or evolutionary algorithms to improve the ability of robots to react to unforeseen changes [33], [43].

3.1.2. Main Challenges

The first major challenge is to endow robots with a stable situation awareness in open and dynamic environments. This covers both the state estimation of the robot itself as well as the perception/representation of the environment. Both problems have been claimed to be solved but it is only the case for static environments [42].

In the LARSEN team, we aim at deployment in environments shared with humans which directly translates into dynamic objects that degrade both the mapping and localization, especially in cluttered spaces. Moreover, when robots stay longer in the environment than for the acquisition of a snapshot map, they have to face structural changes, such as the displacement of a piece of furniture or the opening or closing of a door. The current approach is to simply update an implicitly static map with all observations with no attempt at distinguishing the suitable changes. For localization in not-too-cluttered or not-too-empty environments, this is generally sufficient as a significant fraction of the environment should remain stable. But for life-long autonomy, and in particular navigation, the quality of the map, and especially the knowledge of the stable parts, is primordial.

A second major obstacle to move robots outside of labs and factories is their fragility: current robots often break in a few hours, if not a few minutes. This fragility mainly stems from the overall complexity of robotics systems, which involve many actuators, many sensors, and complex decisions, and from the diversity of situations that robots can encounter. Low-cost robots exacerbate this issue because they can be broken in many ways (high-quality material is expensive), because they have low self-sensing abilities (sensors are expensive and increase the overall complexity), and because they are typically targeted towards non-controlled environments (e.g., houses, by opposition to factories, in which robots are protected from most unexpected events). More generally, this fragility is a symptom of the lack of adaptive abilities in current robots.

3.1.3. Angle of Attack

To solve the state estimation problem, our approach is to combine classical estimation filters (Extended Kalman Filters, Unscented Kalman Filters, or particle filters) with a Bayesian reasoning model in order to internally simulate various configurations of the robot in its environment. This should allow for adaptive estimation that can be used as one aspect of long-term adaptation. To handle dynamic and structural changes in an environment, we aim at assessing, for each piece of observation, whether it is static or not.

We also plan to address active sensing to improve the situation awareness of robots. Literally, active sensing is the fact for an interacting agent – equipped with sensors and effectors – to act so as to control what it senses from its environment. The objective is typically to acquire information about this environment. A good example of such an agent is a mobile robot operating in an unknown or a partially known dynamic environment in order to acquire information about some studied phenomena. Active sensing has applications to autonomous data collection, environment monitoring, sound sources localisation or robotic exploration missions. A formalism for representing and solving active sensing problems has already been proposed by members of the team [32] and we will aim to use it to formalize decision making problems of improving situation awareness.

Situation awareness of robots can also be tackled by cooperation whether it be between robots or between robots and sensors in the environment (led out intelligent spaces) or between robots and humans. We envision here robots with symbiotic autonomy i.e., robots that are aware of their limitations and proactively ask for help from humans, other robots or sensors. This will be addressed and formalized in the framework of distributed sensing. Distributed sensing may include active sensing, but it differs in the fact that a large number of sensors are spread in the environment. Due to recent advances in the development of sensor networks and the rapid growth of the Internet of Things, it is simple, today, to deploy a distributed sensing system. This is why the combination of environmental sensors and robots is especially appealing for monitoring complex environments, cluttered with obstacles and populated by humans. This is in rupture with classical robotics, in which robots are conceived as self-contained: they are composed of actuators, sensors and computers and are designed to carry out a multitude of tasks in full autonomy: localisation, mapping, navigation, interaction, etc. But, in order to cope with as diverse environments as possible, these classical robots use precise, expensive and specialized sensors such as for example 3D laser range finders. However, the cost of these sensors prohibits their use in large-scale deployments for service or assistance applications. Furthermore, when all sensors are on the robot, they share the same point of view on the environment with all that it entails in terms of perception complexity. Therefore, we propose to complement a cheaper robot with sensors distributed in a target environment, gathering the information flow in a usable representation for robots, controlling active sensors such as robots and mobile sensors (camera mounted on a pan-tilt unit). This is an emerging research direction that shares some of the problematics of multi-robot operation – such as synchronization and collaborative planning or swarm intelligence – and sensor networks – such as calibration. We are therefore collaborating with other teams at Inria that address the issue of communication and interoperability.

To address the fragility problem, the traditional approach is to first diagnose the situation, then use a planning algorithm to create/select a contingency plan. The main challenge here is to take uncertainties into account both in the diagnosis and in the planning, a challenge naturally suited for Bayesian methods [45].

An alternative approach is to skip the diagnosis and let the robot discover by trial and error a behavior that works in spite of the damage, that is, to use a reinforcement learning algorithm [54], [43]. This approach could be especially appropriate for low-cost autonomous robots because diagnostic procedures require expensive proprioceptive sensors, and because the possible faults in a complex, autonomous robot that works in an open and dynamic environments are almost infinite. However, current reinforcement learning algorithms require hundreds of trials/episodes to learn a single, often simplified, task [43], which makes them impossible to use for real robots and more ambitious tasks. **We therefore need to design new trial-and-error algorithms that will allow robots to learn with a much smaller number of trials (typically, a dozen).** We think the key idea is to guide online learning on the physical robot with dynamic simulations. In particular, we will work on combining the exploration abilities of evolutionary algorithms [35] with the convergence speed of gradient-free, continuous, model-based optimization algorithms, like Bayesian Optimization [47], [49]. In our recent work, we successfully mixed evolutionary search in simulation, physical tests on the robot, and machine learning to allow a robot to recover from physical damages [44], [2]. We will continue in this direction.

Another approach to address fragility is to deploy several robots or a swarm of robots or make robots evolve in an active environment. We will consider several paradigms such as (1) those inspired from collective natural phenomena in which the environment plays an active role for coordinating the activity of a huge number of biological entities such as ants; (2) those based on online learning [41]. We envision to transfer our knowledge

of such phenomenon to engineer new artificial devices such as an intelligent floor (which is in fact a spatially distributed network in which each node can sense, compute and communicate with contiguous nodes and can interact with moving entities on top of it) in order to assist people and robots (see the principle in [52], [41] [18]).

3.2. Natural Interaction with Robotic Systems

3.2.1. Scientific Context

Interaction with the environment is the primordial requirement for an autonomous robot: the robot must rely on measurements from its onboard sensors and, when available, can benefit from exteroceptive sensors distributed in the environment (e.g., external cameras, motion detectors, beacons) in order to model its surrounding and plan its actions based on its status. In this sense, interaction with the environment also includes interaction between the robot and a sensorized environment (sometimes called “smart”, “connected”, or “robotized”) or interaction between the human and this robotics environment. Taking decisions when multiple sensors are spread in such environments is still an open question. In many applications, this requires the capability of the robot to localize itself while moving, and for the environment to fuse the information from its multiple distributed sensors to track the behaviors of robots and humans, analyzing their actions and predicting their intent.

Predicting the evolution of the environment and of the different agents (robots and humans) that populate it, is of primary importance for taking valuable decision in dynamical environments. However, this is still a challenging problem, especially because we lack robust predictive models of human behavior. Using environmental sensors capable to extract main human social or physical signals (e.g., posture or gaze) is a way to simplify the problem for a robot. Putting together information from different sensors and viewpoints is beneficial for robots understanding complex scenes but often significantly increases the complexity of the data and of the representations that can be formed of the environment. At the same time, we aim at being able to control robots or mobile sensors, which means deciding, at each time instant, what to do. A critical constraint is the uncertainty arising both from the incomplete knowledge of the environment and the other agents (typically humans) that share this environment, and from the intrinsic noise of sensors and actuators.

When working in proximity of or directly with humans, robots must be capable of interacting safely with them, which calls upon a mixture of physical and social skills. In particular, robots working outside labs must exhibit the necessary social skills that allow them to interact with people that are not robotics experts. People operating industrial robots are usually specialized operators that receive a proper training for programming and operating the machines [31]. In contrast, the potential end-users of robots for service or personal assistance are usually not familiar with new technologies and robots [46]. To introduce robots in these contexts, the robot must be accepted as a reliable, trustworthy and efficient partner; it must be able to be used by people that are not skilled robotics experts [58], therefore be endowed with the necessary social skills; it must be capable to interact physically with humans, a skill that calls upon its online learning, control and adaptation skills. Despite the growing interest of the robotics community for physical Human-Robot Interaction (HRI) [34], social and collaborative HRI [56], [51], there are few examples in the literature about incorporating human signals in the control of movement and interaction forces. There are also very few examples of whole-body control of robot movement that takes into account human feedback [39]. In psychology, the literature analyzing the social and cognitive aspects of interaction is notable [36], [56]. Sadly, as discussed by [53], most HRI studies focus on verbal communication, and there are only few studies about dyadic interaction with physical contacts with robots. On the contrary, **applications such as assistance robotics require a deeper knowledge of the intertwined exchange of social and physical signals to provide suitable robot controllers.**

3.2.2. Main Challenges

We are here interested in building the bricks for a situated Human-Robot Interaction (HRI) addressing both the physical and social dimension of the close interaction, and the cognitive aspects related to the analysis and interpretation of human movement and activity.

The combination of physical and social signals into the robot control is a crucial investigation for assistance robots [55] and robotic co-workers [51]. A major obstacle is the control of physical interaction (precisely, the control of contact forces) between the robot and the human, while both partners are moving. In mobile robots, this problem is usually addressed by planning the robot movement taking into account the human as an obstacle or as a target, then delegating the execution of this “high-level” motion to whole-body controllers, where a mixture of weighted tasks is used to account for the robot balance, constraints and desired end-effectors trajectories [37].

The first challenge is to make these controllers easier to deploy in real robotics systems, as currently they require a lot of tuning and can become very complex to handle the interaction with unknown dynamical systems such as humans. Here, the key is to combine machine learning techniques with such controllers.

The second challenge is to make the robot react and adapt online to the human feedback, exploiting the whole set of measurable verbal and non-verbal signals that humans naturally produce during a physical or social interaction. Technically, this means finding the optimal policy that adapts the robot controllers online, taking into account feedback from the human. Here, we need to carefully identify the significant feedback signals or some metrics of human feedback. In real-world conditions (i.e., outside the research laboratory environment) the set of signals is technologically limited by the robot’s and environmental sensors and the onboard processing capabilities.

The third challenge is for a robot to be able to identify and track people on board. The motivation is to be able to estimate online either the position, the posture, or even moods and intentions of persons surrounding the robot. The main challenge is to be able to do that online, in real-time and in cluttered environments.

3.2.3. *Angle of Attack*

Our key idea is to exploit the physical and social signals produced by the human during the interaction with the robot and the environment in controlled conditions, to learn simple models of human behavior. Consequently, use these models to optimize the robot movements and actions. In a first phase, we will exploit the human physical signals (e.g., posture and force measurements) to identify the elementary posture tasks during balance and physical interaction. The identified model will be used to optimize the robot whole-body control, as a prior knowledge that is used to improve both the robot balance and the control of the interaction forces. Technically, we will combine weighted and prioritized controllers with stochastic optimization techniques. To adapt online the control of physical interaction and make it possible with human partners that are not robotics experts, we will exploit verbal and non-verbal signals (e.g., gaze, touch, prosody). The idea here is to estimate online from these signals the human intent along with some inter-individual factors that the robot can exploit to adapt its behavior, maximizing the engagement and acceptability during the interaction.

Another promising approach already investigated in LARSEN team is the capability for a robot and/or an intelligent space to localize humans in its surrounding environment and to understand their activities. This is an important issue to handle both for safe and efficient human-robot interaction.

Simultaneous Tracking and Activity Recognition (STAR) [57] is an approach we want to develop. The activity of a person is highly correlated with its position and this approach aims at combining tracking and activity recognition to benefit one from another. By tracking the individual, the system may help infer its possible activity, while by estimating the activity of the individual, the system may have a better prediction of its possible future positions (which can be very effective in case of occlusion). This direction has been tested with simulator and particle filters [40] and one promising direction would be to couple STAR with decision making formalisms like partially observable Markov decision processes, POMDPs). This would allow to formalize problems such as deciding which action to take given an estimate of the human location and activity. This could also formalize other problems linked to the active sensing direction of the team: how the robotic system might choose its actions in order to have a better estimate of the human location and activity (for instance by moving in the environment or by changing the orientation of its cameras)?

Another issue we want to address is robotic human body pose estimation. Human body pose estimation consists of tracking body parts by analyzing a sequence of input images from single or multiple cameras.

Human posture analysis is of high value for human robot interaction or activity recognition. However, even if the arrival of new sensors like RGB-D cameras has simplified the problem, it still poses a great challenge, especially if we want to do it online, on a robot and in realistic world conditions (cluttered environment). This is even worse for a robot to bring together different capabilities both at the perception and navigation level [38]. This will be tackled through different techniques going from Bayesian state estimation (particle filtering), learning, active and distributed sensing.

MADYNES Project-Team

3. Research Program

3.1. Evolutionary needs in network and service management

The foundation of the MADYNES research activity is the ever increasing need for automated monitoring and control within networked environments. This need is mainly due to the increasing dependency of both people and goods towards communication infrastructures as well as the growing demand towards services of higher quality. Because of its strategic importance and crucial requirements for interoperability, the management models were constructed in the context of strong standardization activities by many different organizations over the last 15 years. This has led to the design of most of the paradigms used in today's deployed approaches. These paradigms are the Manager/Agent interaction model, the Information Model paradigm and its container, together with a naming infrastructure called the Management Information Base. In addition to this structure, five functional areas known under Fault, Configuration, Accounting, Performance and Security are associated to these standards.

While these models were well suited for the specific application domains for which they were designed (telecommunication networks or dedicated protocol stacks), they all show the same limits. Especially they are unable:

1. to deal with any form of dynamicity in the managed environment,
2. to master the complexity, the operating mode and the heterogeneity of the emerging services,
3. to scale to new networks and service environments.

These three limits are observed in all five functional areas of the management domain (fault, configuration, accounting, performance and security) and represent the major challenges when it comes to enable effective automated management and control of devices, networks and services in the next decade.

MADYNES addresses these challenges by focusing on the design of management models that rely on inherently dynamic and evolving environments. The project is centered around two core activities. These activities are, as mentioned in the previous section, the design of an autonomous management framework and its application to three of the standard functional areas namely security, configuration and performance.

3.2. Autonomous management

3.2.1. *Models and methods for a self-management plane*

Self organization and automation are fundamental requirements within the management plane in today's dynamic environments. It is necessary to automate the management processes and enable management frameworks to operate in time sensitive evolving networks and service environments. The automation of the organization of devices, software components, networks and services is investigated in many research projects and has already led to several solution proposals. While these proposals are successful at several layers, like IP auto-configuration or service discovery and binding facilities, they did not enhance the management plane at all. For example, while self-configuration of IP devices is commonplace, no solution exists that provides strong support to the management plane to configure itself (e.g. finding the manager to which an agent has to send traps or organizing the access control based on locality or any other context information). So, this area represents a major challenge in extending current management approaches so that they become self-organized.

Our approach is bottom-up and consists in identifying those parameters and framework elements (manager data, information model sharing, agent parameters, protocol settings, ...) that need dynamic configuration and self-organization (like the address of a trap sink). For these parameters and their instantiation in various management frameworks (SNMP, Netconf, WBEM, ...), we investigate and elaborate novel approaches enabling fully automated setup and operation in the management plane.

3.2.2. *Design and evaluation of P2P-based management architectures*

Over the last years, several models have emerged and gained wide acceptance in the networking and service world. Among them, the overlay networks together with the P2P paradigms appear to be very promising. Since they rely mainly on fully decentralized models, they offer excellent fault tolerance and have a real potential to achieve high scalability. Mainly deployed in the content delivery and the cooperation and distributed computation disciplines, they seem to offer all features required by a management framework that needs to operate in a dynamic world. This potential however needs an in depth investigation because these models have also many characteristics that are unusual in management (e.g. a fast and uncontrolled evolution of the topology or the existence of a distributed trust relationship framework rather than a standard centralized security framework).

Our approach envisions how a complete redesign of a management framework is done given the characteristics of the underlying P2P and overlay services. Among the topics of interest we study the concept of management information and operations routing within a management overlay as well as the distribution of management functions in a multi-manager/agent P2P environment. The functional areas targeted in our approach by the P2P model are network and service configuration and distributed monitoring. The models are to be evaluated against highly dynamic frameworks such as ad-hoc environments (network or application level) and mobile devices.

3.2.3. *Integration of management information*

Representation, specification and integration of management information models form a foundation for network and service management and remains an open research domain. The design and specification of new models is mainly driven by the appearance of new protocols, services and usage patterns. These need to be managed and exposed through well designed management information models. Integration activities are driven by the multiplication of various management approaches. To enable automated management, these approaches need to inter-operate which is not the case today.

The MADYNES approach to this problem of modeling and representation of management information aims at:

1. enabling application developers to establish their management interface in the same workspace, with the same notations and concepts as the ones used to develop their application,
2. fostering the use of standard models (at least the structure and semantics of well defined models),
3. designing a naming structure that allows the routing of management information in an overlay management plane, and
4. evaluating new approaches for management information integration especially based on management ontologies and semantic information models.

3.2.4. *Modeling and benchmarking of dynamic networks*

The impact of a management approach on the efficiency of the managed service is highly dependent on three factors:

- the distribution of the considered service and their associated management tasks,
- the management patterns used (e.g. monitoring frequency, granularity of the management information considered),
- the cost in terms of resources these considered functions have on the managed element (e.g. method call overhead, management memory footprint).

MADYNES addresses this problem from multiple viewpoints: communication patterns, processing and memory resources consumption. Our goal is to provide management patterns combining optimized management technologies so as to optimize the resources consumed by the management activity imposed by the operating environment while ensuring its efficiency in large dynamic networks.

3.3. Functional areas

3.3.1. Security management

Securing the management plane is vital. While several proposals are already integrated in the existing management frameworks, they are rarely used. This is due to the fact that these approaches are completely detached from the enterprise security framework. As a consequence, the management framework is “managed” separately with different models; this represents a huge overhead. Moreover the current approaches to security in the management plane are not inter-operable at all, multiplying the operational costs in a heterogeneous management framework.

The primary goal of the research in this activity is the design and the validation of a security framework for the management plane that will be open and capable to integrate the security services provided in today’s management architectures. Management security interoperability is of major importance in this activity.

Our activity in this area aims at designing a generic security model in the context of multi-party / multi-technology management interactions. Therefore, we develop research on the following directions:

1. Abstraction of the various access control mechanisms that exist in today’s management frameworks. We are particularly interested in extending these models so that they support event-driven management, which is not the case for most of them today.
2. Extension of policy and trust models to ease and to ensure coordination among managers towards one agent or a subset of the management tree. Provisional policies are of great interest to us in this context.
3. Evaluation of the adequacy of key distribution architectures to the needs of the management plane as well as selecting reputation models to be used in the management of highly dynamic environments (e.g. multicast groups, ad-hoc networks).

A strong requirement towards the future generic model is that it needs to be instantiated (with potential restrictions) into standard management platforms like SNMP, WBEM or Netconf and to allow interoperability in environments where these approaches coexist and even cooperate. A typical example of this is the security of an integration agent which is located in two management worlds.

Since 2006 we have also started an activity on security assessment. The objective is to investigate new methods and models for validating the security of large scale dynamic networks and services. The first targeted service is VoIP.

3.3.2. Configuration: automation of service configuration and provisioning

Configuration covers many processes which are all important to enable dynamic networks. Within our research activity, we focus on the operation of tuning the parameters of a service in an automated way. This is done together with the activation topics of configuration management and the monitoring information collected from the underlying infrastructure. Some approaches exist today to automate part of the configuration process (download of a configuration file at boot time within a router, on demand code deployment in service platforms). While these approaches are interesting they all suffer from the same limits, namely:

1. they rely on specific service life cycle models,
2. they use proprietary interfaces and protocols.

These two basic limits have high impacts on service dynamics in a heterogeneous environment.

We follow two research directions in the topic of configuration management. The first one aims at establishing an abstract life-cycle model for either a service, a device or a network configuration and to associate with this model a generic command and programming interface. This is done in a way similar to what is proposed in the area of call control in initiatives such as Parlay or OSA.

In addition to the investigation of the life-cycle model, we work on technology support for distributing and exchanging configuration management information. Especially, we investigate policy-driven approaches for representing configurations and constraints while we study XML-based protocols for coordinating distribution and synchronization. Off and online validation of configuration data is also part of this effort.

3.3.3. Performance and availability monitoring

Performance management is one of the most important and deployed management function. It is crucial for any service which is bound to an agreement about the expected delivery level. Performance management needs models, metrics, associated instrumentation, data collection and aggregation infrastructures and advanced data analysis algorithms.

Today, a programmable approach for end-to-end service performance measurement in a client server environment exists. This approach, called Application Response Measurement (ARM) defines a model including an abstract definition of a unit of work and related performance records; it offers an API to application developers which allows easy integration of measurement within their distributed application. While this approach is interesting, it is only a first step toward the automation of performance management.

We are investigating two specific aspects. First we are working on the coupling and possible automation of performance measurement models with the upper service level agreement and specification levels. Second we are working on the mapping of these high level requirements to the lower level of instrumentation and actual data collection processes available in the network. More specifically we are interested in providing automated mapping of service level parameters to monitoring and measurement capabilities. We also envision automated deployment and/or activation of performance measurement sensors based on the mapped parameters. This activity also incorporates self-instrumentation (and when possible on the fly instrumentation) of software components for performance monitoring purpose.

MAGRIT Project-Team

3. Research Program

3.1. Matching and 3D tracking

One of the most basic problems currently limiting AR applications is the registration problem. The objects in the real and virtual worlds must be properly aligned with respect to each other, or the illusion that the two worlds coexist will be compromised.

As a large number of potential AR applications are interactive, real time pose computation is required. Although the registration problem has received a lot of attention in the computer vision community, the problem of real-time registration is still far from being a solved problem, especially for unstructured environments. Ideally, an AR system should work in all environments, without the need to prepare the scene ahead of time, independently of the variations in experimental conditions (lighting, weather condition,...) which may exist between the application and the time the model of the scene was acquired.

For several years, the MAGRIT project has been aiming at developing on-line and marker-less methods for camera pose computation. The main difficulty with on-line tracking is to ensure robustness of the process over time. For off-line processes, robustness is achieved by using spatial and temporal coherence of the considered sequence through move-matching techniques. To get robustness for open-loop systems, we have investigated various methods, ranging from statistical methods to the use of hybrid camera/sensor systems. Many of these methods are dedicated to piecewise-planar scenes and combine the advantage of move-matching methods and model-based methods. In order to reduce statistical fluctuations in viewpoint computation, which lead to unpleasant jittering or sliding effects, we have also developed model selection techniques which allow us to noticeably improve the visual impression and to reduce drift over time. Another line of research which has been considered in the team to improve the reliability and the robustness of pose algorithms is to combine the camera with another form of sensor in order to compensate for the shortcomings of each technology.

The success of pose computation over time largely depends on the quality of the matching at the initialization stage. Indeed, the current image may be very different from the appearances described in the model both on the geometrical and the photometric sides. Research is thus conducted in the team on the use of probabilistic methods to establish robust correspondences of features. The use of *a contrario* has been investigated to achieve this aim [6]. We especially addressed the complex case of matching in scenes with repeated patterns which are common in urban scenes. We are also investigating the problem of matching images taken from very different viewpoints which is central for the re-localization issue in AR. Within the context of a scene model acquired with structure from motion techniques, we are currently investigating the use of viewpoint simulation in order to allow successful pose computation even if the considered image is far from the positions used to build the model [21].

Recently, the issue of tracking deformable objects has gained importance in the team. This topic is mainly addressed in the context of medical applications through the design of bio-mechanical models guided by visual features [1]. We have successfully investigated the use of such models in laparoscopy, with a vascularized model of the liver and with an hyper-elastic model for tongue tracking in ultrasound images. However, these results have been obtained so far in relatively controlled environments, with non pathological cases. When clinical routine applications are to be considered, many parameters and considerations need to be taken into account. Among the problems that need to be addressed are more realistic model representations, the specification of the range of physical parameters and the need to enforce the robustness of the tracking with respect to outliers, which are common in the interventional context.

3.2. Image-based Modeling

Modeling the scene is a fundamental issue in AR for many reasons. First, pose computation algorithms often use a model of the scene or at least some 3D knowledge on the scene. Second, effective AR systems require a model of the scene to support interactions between the virtual and the real objects such as occlusions, lighting reflections, contacts...in real-time. Unlike pose computation which has to be computed in a sequential way, scene modeling can be considered as an off-line or an on-line problem depending on the requirements of the targeted application. Interactive in-situ modeling techniques have thus been developed with the aim to enable the user to define what is relevant at the time the model is being built during the application. On the other hand, we also proposed off-line multimodal techniques, mainly dedicated to AR medical applications, with the aim to obtain realistic and possibly dynamic models of organs suitable for real-time simulation.

In-situ modeling

In-situ modeling allows a user to directly build a 3D model of his/her surrounding environment and verify the geometry against the physical world in real-time. This is of particular interest when using AR in unprepared environments or building scenes that either have an ephemeral existence (e.g., a film set) or cannot be accessed frequently (e.g., a nuclear power plant). We have especially investigated two systems, one based on the image content only and the other based on multiple data coming from different sensors (camera, inertial measurement unit, laser rangefinder). Both systems use the camera-mouse principle [4] (i.e., interactions are performed by aiming at the scene through a video camera) and both systems have been designed to acquire polygonal textured models, which are particularly useful for camera tracking and object insertion in AR.

Multimodal modeling for real-time simulation

With respect to classical AR applications, AR in medical context differs in the nature and the size of the data which are available: a large amount of multimodal data is acquired on the patient or possibly on the operating room through sensing technologies or various image acquisitions [2]. The challenge is to analyze these data, to extract interesting features, to fuse and to visualize this information in a proper way. Within the MAGRIT team, we address several key problems related to medical augmented environments. Being able to acquire multimodal data which are temporally synchronized and spatially registered is the first difficulty we face when considering medical AR. Another key requirement of AR medical systems is the availability of 3D (+t) models of the organ/patient built from images, to be overlaid onto the users' view of the environment.

Methods for multimodal modeling are strongly dependent on the image modalities and the organ specificities. We thus only address a restricted number of medical applications –interventional neuro-radiology, laparoscopic surgery, Augmented Head project– for which we have a strong expertise and close relationships with motivated clinicians. In these applications, our aim is to produce realistic models and then realistic simulations of the patient to be used for surgeon's training or patient's re-education/learning.

One of our main applications is about neuroradiology. For the last 20 years, we have been working in close collaboration with the neuroradiology laboratory (CHU-University Hospital of Nancy) and GE Healthcare. As several imaging modalities are now available in an intraoperative context (2D and 3D angiography, MRI, ...), our aim is to develop a multi-modality framework to help therapeutic decision and treatment.

We have mainly been interested in the effective use of a multimodality framework in the treatment of arteriovenous malformations (AVM) and aneurysms in the context of interventional neuroradiology. The goal of interventional gestures is to guide endoscopic tools towards the pathology with the aim to perform embolization of the AVM or to fill the aneurysmal cavity by placing coils. We have proposed and developed multimodality and augmented reality tools which make various image modalities (2D and 3D angiography, fluoroscopic images, MRI, ...) cooperate in order to help physicians in clinical routine. One of the successes of this collaboration is the implementation of the concept of *augmented fluoroscopy*, which helps the surgeon to guide endoscopic tools towards the pathology. Lately, in cooperation with the team MIMESIS, we have proposed new methods for implicit modeling of the vasculature with the aim of obtaining near real-time simulation of the coil deployment in the aneurysm [8]. These works open the way towards near real-time patient-based simulations of interventional gestures both for training and for planning.

3.3. Parameter estimation

Many problems in computer vision or image analysis can be formulated in terms of parameter estimation from image-based measurements. This is the case of many problems addressed in the team such as pose computation or image-guided estimation of 3D deformable models. Often traditional robust techniques which take into account the covariance on the measurements are sufficient to achieve reliable parameter estimation. However, depending on their number, their spatial distribution and the uncertainty on these measurements, some problems are very sensitive to noise and there is a considerable interest in considering how parameter estimation could be improved if additional information on the noise is available. Another common problem in our field of research is the need to estimate constitutive parameters of the models, such as (bio)-mechanical parameters for instance. Direct measurement methods are destructive and elaborating image based methods is thus highly desirable. Besides designing appropriate estimation algorithms, a fundamental question is to understand what group of parameters under study can be reliably estimated from a given experimental setup.

This line of research is relatively new in the team. One of the challenges is to improve image-based parameter estimation techniques considering sensor noise and specific image formation models. In a collaboration with the Pascal Institute (Clermont Ferrand), metrological performance enhancement for experimental solid mechanics has been addressed through the development of dedicated signal processing methods. In the medical field, specific methods based on an adaptive evolutionary optimization strategy have been designed for estimating respiratory parameters [7]. In the context of designing realistic simulators for neuroradiology, we are now considering how parameters involved in the simulation could be adapted to fit real images.

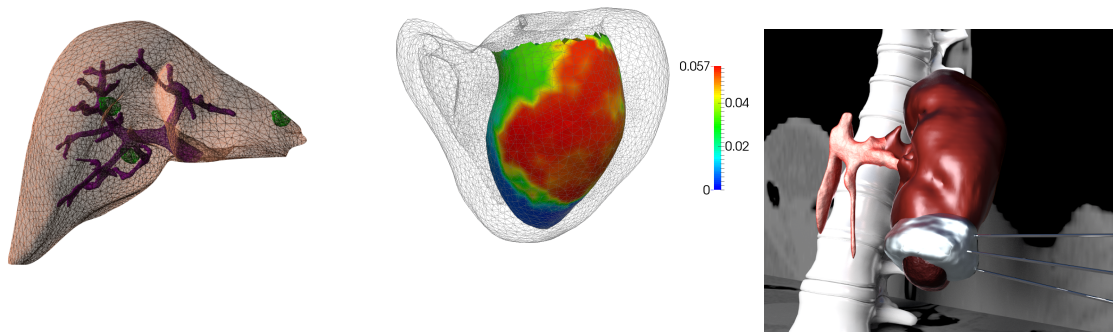
MIMESIS Team

3. Research Program

3.1. Real-Time Patient-Specific Computational Models

The main objective of this scientific challenge is the modeling of the biomechanics and physiology of certain organs under various stimuli. This requires describing different biophysical phenomena such as soft-tissue deformation, fluid dynamics, electrical propagation, or heat transfer. These models help simulate the impact of certain therapies (such as cryosurgery or radio-frequency ablation), but also represent the behavior of complex organs such as the brain, the liver or the heart. A common requirement across these developments is the need for (near) real-time computation and the ability to take into account for patient-specific characteristics.

An important part of our research was dedicated to the development of new **accurate models that remain compatible with real-time computation**. Such advanced models do not only permit to increase the realism of future training systems, but they act as a bridge toward the development of patient-specific preoperative planning as well as augmented reality tools for the operating room. Yet, patient-specific planning or per-operative guidance also requires the models to be **parametrized with patient-specific biomechanical data**. The objective in this area is related to the study of hyper-elastic models and their validation for a range of tissues. Preliminary work in this area has been done through two collaborations, one with the biomechanical lab in Lille (LML) with which we have a joint PhD student, and the biomechanics group from the ICube laboratory in Strasbourg on the development and validation of liver and kidney models. Another important research topic was related to model reduction through various approaches, such as Proper Generalized Decomposition (PGD). We have already established discussions with the LEGATO team at University of Luxembourg which has very good expertise in this area.



- (a) Patient-specific mechanical model of the liver with its vascular system extracted from Computed Tomography Angiogram, and compatible with real-time simulation
- (b) Simulation of the electrical activity of a human heart from intra-operative depolarization map
- (c) Thermal evolution within a human kidney used in the context of cryoablation

Figure 3. Multi-physics and patient-specific models

We continued our work on cardiac electro-physiology simulation, with a focus on patient-specific adaptation of the model. We also studied the simulation of heat transfer and optimization problems in the context of heat diffusion. This work is a key element of the development of a planning system, such as for cryoablation procedures (Figure 3).

3.2. Adaptive Meshing and Advanced Simulation Technologies

The principal objective of this second challenge is to improve, at the numerical level, the efficiency, robustness, and quality of the simulations. To reach these goals, we followed two main directions: **adaptive meshing** to allow mesh transformations during a simulation and support cuts, local remeshing or dynamic refinement into areas of interest; and **numerical techniques**, such as asynchronous solvers, domain decomposition and model order reduction. Most simulations in the field of biomechanics, physiological modeling, or even computer graphics, are performed using finite element approaches. Such simulations require a discretization of the domain of interest, and this discretization is traditionally made of tetrahedral or hexahedral elements. The topology defined by these elements is also considered constant. The first objective of this work is to jointly develop **advanced topological operations and new finite element approaches that can leverage the use of dynamic topologies**. This covers various topics, such as simulation for cutting, tearing, fracture but also the use of multi-resolution meshes where elements are subdivided into areas where numerical errors need to be kept small [37], [38]. We also continued our work on mixed Finite Element Modeling where both tetrahedra and hexahedra can be used at the same time, allowing an ideal compromise between numerical efficiency and mesh adaptation to complex geometries (Figure 4). This research also includes the study of domain decomposition techniques and other coupling techniques for multi-domain multi-physics simulations.

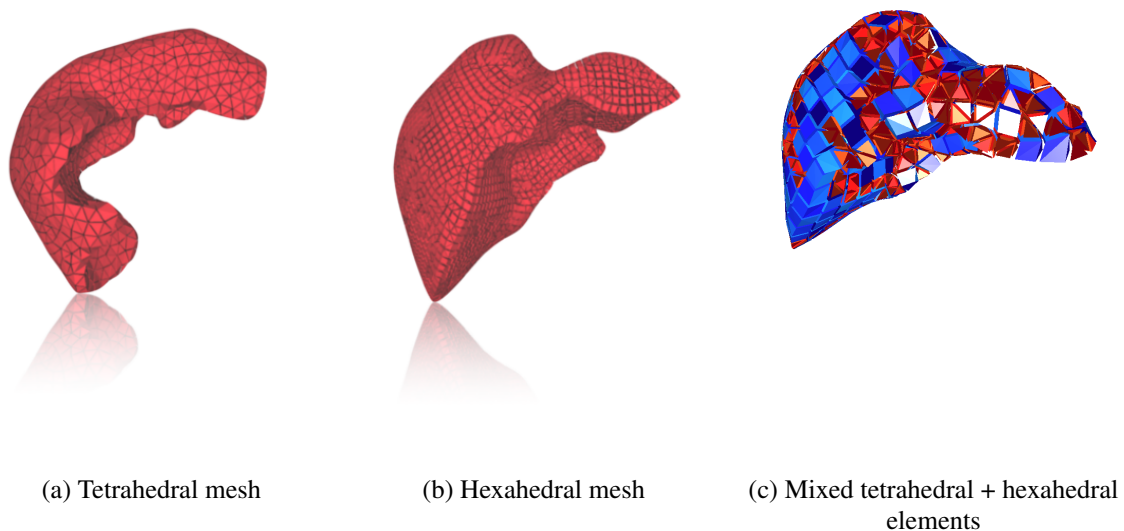


Figure 4. Patient-specific volumetric meshes of the liver

3.3. Image-Driven Simulation

Image-guided simulation is a recent area of research that has the potential to bridge the gap between medical imaging and clinical routine by adapting pre-operative data to the time of the procedure. Several challenges are related to image-guided therapy but the main issue consists in aligning pre-operative images onto patient per-operative data and keep this alignment up-to-date during the procedure. As most procedures deal with soft-tissues, elastic registration techniques are necessary to perform this step. Recently, registration techniques started to account for soft tissue biomechanics using physically-based methods, yet several limitations still hinder the use of image-guided therapy in clinical routine. First, as registration methods become more complex, their computation times increase, thus lacking responsiveness. Second, techniques used for non-rigid registration or deformable augmented reality only “borrow” ideas from continuum mechanics but lack some key elements (such as identification of the rest shape, or definition of the boundary conditions). Also, these

registration or augmented reality problems are highly dependent on the choice of image modality and require investigating some aspects of computer vision or medical image processing. However, if we can properly address these challenges, the combination of a real-time simulation and regular acquisitions of image data during the procedure opens up very interesting possibilities by using data assimilation to better adapt the model to the intra-operative data. In the area of non-rigid registration and augmented reality, we have already demonstrated the benefit of our physics-based approaches. This was applied in particular to the problem of organ tracking during surgery (Figure 5) and led to several key publications [35], [36], [34] and awards (best paper at ISMAR 2013, second best paper at IPCAI 2014). We continued this work with an emphasis on robustness to uncertainty and outliers in the information extracted in real-time from image data. We also improved our computer vision techniques, in particular to guarantee a very accurate initial registration of the pre-operative model onto the per-operative surface patch extracted from monocular or stereo laparoscopic cameras.

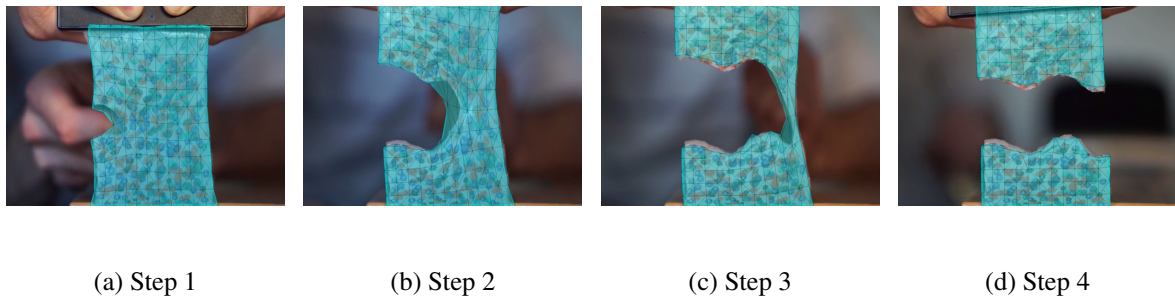


Figure 5. An augmented elastic object undergoing large deformations and topological changes. The computation of the physics-based deformation, the cut detection and the topological modification of the underlying volumetric model are all performed in real-time.

The use of simulation in the context of image-guided therapy can be extended in several other ways. A direction we particularly want to address is the **combined use of simulation and X-ray imaging during interventional radiology procedures**. Whether it is for percutaneous procedures or catheterization, the task of the simulation is to provide a short-term (1 to 5 seconds) prediction of the needle or catheter position. **Using information extracted from the image, the parameters of the simulation can be assimilated** (using methods such as unscented Kalman filters), so that the simulation progressively matches the real data in order to reduce uncertainties. We have already started to create a flexible framework integrating the real-time soft-tissue simulation and state-of-the-art methods of data assimilation and filtering. The reduced-order stochastic filtering is a computationally efficient improvement over traditional computationally expensive **approaches which fits well the real-time and patient-specific requirements** arising from our per-operative context.

MULTISPEECH Project-Team

3. Research Program

3.1. Introduction

MULTISPEECH is structured along three research directions that are associated to the previously described challenges: explicit modeling of speech, statistical modeling of speech, and uncertainty in speech processing.

3.2. Explicit Modeling of Speech Production and Perception

Speech signals are the consequence of the deformation of the vocal tract under the effect of the movements of the articulators (jaw, lips, tongue, ...) to modulate the excitation signal produced by the vocal cords or air turbulence. These deformations are visible on the face (lips, cheeks, jaw) through the coordination of different orofacial muscles and skin deformation induced by the latter. These deformations may also express different emotions. We should note that human speech expresses more than just phonetic content, to be able to communicate effectively. In this project, we address the different aspects related to speech production from the modeling of the vocal tract up to the production of expressive audiovisual speech. Phonetic contrasts used by the phonological system of any language result from constraints imposed by the nature of the human speech production apparatus. For a given language these contrasts are organized so as to guarantee that human listeners can identify (categorize) sounds robustly. The study of the categorization of sounds and prosody thus provides a complementary view on speech signals by focusing on the discrimination of sounds by humans, particularly in the context of language learning.

3.2.1. *Articulatory modeling*

Modeling speech production is a major issue in speech sciences. Acoustic simulation makes the link between articulatory and acoustic domains. Unfortunately this link cannot be fully exploited because there is almost always an acoustic mismatch between natural and synthetic speech generated with an articulatory model approximating the vocal tract. However, the respective effects of the geometric approximation, of the fact of neglecting some cavities in the simulation, of the imprecision of some physical constants and of the dimensionality of the acoustic simulation are still unknown. Hence, the first objective is to investigate the origin of the acoustic mismatch by designing more precise articulatory models, developing new methods to acquire tridimensional Magnetic Resonance Imaging (MRI) data of the entire vocal tract together with denoised speech signals, and evaluating several approaches of acoustic simulation. The articulatory data acquisition relies on a head-neck antenna at Nancy Hospital to acquire MRI of the vocal tract, and on the articulograph Carstens AG501 available in the laboratory.

Up to now, acoustic-to-articulatory inversion has been addressed as an instantaneous problem, articulatory gestures being recovered by concatenating local solutions. The second objective is thus to investigate how more elaborated strategies (a syllabus of primitive gestures, articulatory targets. . .) can be incorporated in the acoustic-to-articulatory inversion algorithms to take into account dynamic aspects.

3.2.2. *Expressive acoustic-visual synthesis*

Speech is considered as a bimodal communication means; the first modality is audio, provided by acoustic speech signals and the second one is visual, provided by the face of the speaker. In our approach, the Acoustic-Visual Text-To-Speech synthesis (AV-TTS) is performed simultaneously with respect to its acoustic and visible components, by considering a bimodal signal comprising both acoustic and visual channels. A first AV-TTS system was developed resulting in a talking head; the system relied on 3D-visual data and on an extension of our acoustic-unit concatenation text-to-speech synthesis system (SoJA). An important goal is to provide an audiovisual synthesis that is intelligible, both acoustically and visually. Thus, we continue working on adding visible components of the head through a tongue model and a lip model. We will also improve the TTS engine to increase the accuracy of the unit selection simultaneously into the acoustic and visual domains. To acquire the facial data, we consider using a marker-less motion capture system using a kinect-like system with a face tracking software, which constitutes a relatively low-cost alternative to the Vicon system.

Another challenging research goal is to add expressivity in the AV-TTS. The expressivity comes through the acoustic signal (prosody aspects) and also through head and eyebrow movements. One objective is to add a prosodic component in the TTS engine in order to take into account some prosodic entities such as emphasis (to highlight some important key words). One intended approach will be to explore an expressivity measure at sound, syllable and/or sentence levels that describes the degree of perception or realization of an expression/emotion (audio and 3D domain). Such measures will be used as criteria in the selection process of the synthesis system. To tackle the expressivity issue we will also investigate Hidden Markov Model (HMM) based synthesis which allows for easy adaption of the system to available data and to various conditions.

3.2.3. Categorization of sounds and prosody for native and non-native speech

Discriminating speech sounds and prosodic patterns is the keystone of language learning whether in the mother tongue or in a second language. This issue is associated with the emergence of phonetic categories, i.e., classes of sounds related to phonemes and prosodic patterns. The study of categorization is concerned not only with acoustic modeling but also with speech perception and phonology. Foreign language learning raises the issue of categorizing phonemes of the second language given the phonetic categories of the mother tongue. Thus, studies on the emergence of new categories, whether in the mother tongue (for people with language deficiencies) or in a second language, must rely upon studies on native and non-native acoustic realizations of speech sounds and prosody, and on perceptual experiments. Concerning prosody, studies are focused on native and non-native realizations of modalities (e.g., question, affirmation, command, ...), as well as non-native realizations of lexical accents and focus (emphasis).

For language learning, the analysis of the prosody and of the acoustic realization of the sounds aims at providing automatic feedbacks to language learners with respect to acquisition of prosody as well as acquisition of a correct pronunciation of the sounds of the foreign language. Concerning the mother tongue we are interested in the monitoring of the process of sound categorization in the long term (mainly at primary school) and its relation with the learning of reading and writing skills [7], especially for children with language deficiencies.

3.3. Statistical Modeling of Speech

Whereas the first research direction deals with the physical aspects of speech and its explicit modeling, this second research direction is concerned by investigating statistical models for speech data. Acoustic models are used to represent the pronunciation of the sounds or other acoustic events such as noises. Whether they are used for source separation, for speech recognition, for speech transcription, or for speech synthesis, the achieved performance strongly depends on the accuracy of these models. At the linguistic level, MULTISPEECH investigates models for handling the context (beyond the few preceding words currently handled by the n -gram models) and evolutive lexicons necessary when dealing with diachronic audio documents. Statistical approaches are also useful for generating speech signals. Along this direction, MULTISPEECH considers voice transformation techniques, with their application to pathological voices, and statistical speech synthesis applied to expressive multimodal speech synthesis.

3.3.1. Source separation

Acoustic modeling is a key issue for automatic speech recognition. Despite the progress made for many years, current speech recognition applications rely on strong constraints (close-talk microphone, limited vocabulary, or restricted syntax) to achieve acceptable performance. The quality of the input speech signals is particularly important and performance degrades quickly with noisy signals. Accurate signal enhancement techniques are therefore essential to increase the robustness of both automatic speech recognition and speech-text alignment systems to noise and non-speech events.

In MULTISPEECH, focus is set on source separation techniques using multiple microphones and/or models of non-speech events. Some of the challenges include getting the most of the new modeling frameworks based on alpha-stable distributions and deep neural networks, combining them with established spatial filtering approaches, modeling more complex properties of speech and audio sources (phase, inter-frame and inter-frequency properties), and exploiting large data sets of speech, noise, and acoustic impulse responses to

automatically discover new models. Beyond the definition of such models, the difficulty will be to design scalable estimation algorithms robust to overfitting, that will integrate into the recently developed FASST [6] and KAM software frameworks.

3.3.2. Linguistic modeling

MULTISPEECH investigates lexical and language models in speech recognition with a focus on improving the processing of proper names and of spontaneous speech. Proper names are relevant keys in information indexing, but are a real problem in transcribing many diachronic spoken documents which refer to data, especially proper names, that evolve over the time. This leads to the challenge of dynamically adjusting lexicons and language models through the use of the context of the documents or of some relevant external information. We also investigate language models defined on a continuous space (through neural network based approaches) in order to achieve a better generalization on unseen data, and to model long-term dependencies. We also want to introduce into these models additional relevant information such as linguistic features, semantic relation, topic or user-dependent information.

Other topics are spontaneous speech and pronunciation lexicons. Spontaneous speech utterances are often ill-formed and frequently contain disfluencies (hesitations, repetitions, ...) that degrade speech recognition performance. Hence the objective of improving the modeling of disfluencies and of spontaneous speech pronunciation variants. Attention will also be set on pronunciation lexicons with respect to non-native speech and foreign names. Non-native pronunciation variants have to take into account frequent miss-pronunciations due to differences between mother tongue and target language phoneme inventories. Proper name pronunciation variants are a similar problem where difficulties are mainly observed for names of foreign origin that can be pronounced either in a French way or kept close to foreign origin native pronunciation.

3.3.3. Speech generation by statistical methods

Voice conversion consists in building a function that transforms a given voice into another one. MULTISPEECH applies voice conversion techniques to enhance pathological voices that result from vocal folds problems, especially esophageal voice or pathological whispered voice. In addition to the statistical aspects of the voice conversion approaches, signal processing is critical for good quality speech output. As the fundamental frequency is chaotic in the case of esophageal speech, the excitation spectrum must be predicted or corrected. Voice conversion techniques are also of interest for text-to-speech synthesis systems as they aim at making possible the generation of new voice corpora (other kind of voice, or same voice with different kind of emotion). Also, in the context of acoustic feedback in foreign language learning, voice modification approaches will be investigated to modify the learner's (or teacher's) voice in order to emphasize the difference between the learner's acoustic realization and the expected realization.

Over the last few years statistical speech synthesis has emerged as an alternative to corpus-based speech synthesis. The announced advantages of the statistical speech synthesis are the possibility to deal with small amounts of speech resources and the flexibility for adapting models (for new emotions or new speaker), however, the quality is not as good as that of the concatenation-based speech synthesis. MULTISPEECH will focus on an hybrid approach, combining corpus-based synthesis, for its high-quality speech signal output, and HMM-based speech synthesis for its flexibility to drive selection, and the main challenge will be on its application to producing expressive audio-visual speech.

3.4. Uncertainty Estimation and Exploitation in Speech Processing

This axis focuses on the uncertainty associated to some processing steps. Uncertainty stems from the high variability of speech signals and from imperfect models. For example, enhanced speech signals resulting from source separation are not exactly the clean original speech signals. Words or phonemes resulting from automatic speech recognition contain errors, and the phone boundaries resulting from automatic speech-text alignment are not always correct, especially in acoustically degraded conditions. Hence it is important to know the reliability of the results and/or to estimate the uncertainty on the results.

3.4.1. Uncertainty and acoustic modeling

Because small distortions in the separated source signals can translate into large distortions in the cepstral features used for speech recognition, this limits the recognition performance on noisy data. One way to address this issue is to estimate the uncertainty on the separated sources in the form of their posterior distribution and to propagate this distribution, instead of a point estimate, through the subsequent feature extraction and speech decoding stages. Although major improvements have been demonstrated in proof-of-concept experiments using knowledge of the true uncertainty, accurate uncertainty estimation and propagation remains an open issue.

MULTISPEECH seeks to provide more accurate estimates of the posterior distribution of the separated source signals accounting for, e.g., posterior correlations over time and frequency which have not been considered so far. The framework of variational Bayesian (VB) inference appears to be a promising direction. Mappings learned on training data and fusion of multiple uncertainty estimators are also explored. The estimated uncertainties is then exploited for acoustic modeling in speech recognition and, in the future, also for speech-text alignment. This approach may later be extended to the estimation of the resulting uncertainty on the acoustic model parameters and the acoustic scores themselves.

3.4.2. Uncertainty and phonetic segmentation

The accuracy of the phonetic segmentation is important in several cases, as for example for the computation of prosodic features, for avoiding incorrect feedback to the learner in computer assisted foreign language learning, or for the post-synchronization of speech with face/lip images. Currently the phonetic boundaries obtained are quite correct on good quality speech, but the precision degrades significantly on noisy and non-native speech. Phonetic segmentation aspects will be investigated, both in speech recognition (i.e., spoken text unknown) and in forced alignment (i.e., when the spoken text is known).

In the same way that combining several speech recognition outputs leads to improved speech recognition performance, MULTISPEECH will investigate the combination of several speech-text alignments as a way of improving the quality of speech-text alignment and of determining which phonetic boundaries are reliable and which ones are not, and also for estimating the uncertainty on the boundaries. Knowing the reliability of the boundaries will also be useful when segmenting speech corpora; this will help deciding which parts of the corpora need to be manually checked and corrected without an exhaustive checking of the whole corpus.

3.4.3. Uncertainty and prosody

Prosody information is also investigated as a means for structuring speech data (determining sentence boundaries, punctuation...) possibly in addition with syntactic dependencies. Structuring automatic transcription output is important for further exploitation of the transcription results such as easier reading after the addition of punctuation, or exploitation of full sentences in automatic translation. Prosody information is also necessary for determining the modality of the utterance (question or not), as well as determining accented words.

Prosody information comes from the fundamental frequency, the duration of the sounds and their energy. Any error in estimating these parameters may lead to a wrong decision. MULTISPEECH will investigate estimating the uncertainty on the duration of the phones (see uncertainty on phonetic boundaries above) and on the fundamental frequency, as well as how this uncertainty shall be propagated in the detection of prosodic phenomena such as accented words, utterance modality, or determination of the structure of the utterance.

NEUROSYS Project-Team

3. Research Program

3.1. Main Objectives

The main challenge in computational neuroscience is the high complexity of neural systems. The brain is a complex system and exhibits a hierarchy of interacting subunits. On a specific hierarchical level, such subunits evolve on a certain temporal and spatial scale. The interactions of small units on a low hierarchical level build up larger units on a higher hierarchical level evolving on a slower time scale and larger spatial scale. By virtue of the different dynamics on each hierarchical level, until today the corresponding mathematical models and data analysis techniques on each level are still distinct. Only few analysis and modeling frameworks are known which link successfully at least two hierarchical levels.

Once having extracted models for different description levels, typically they are applied to obtain simulated activity which is supposed to reconstruct features in experimental data. Although this approach appears straight-forward, it implies various difficulties. Usually the models involve a large set of unknown parameters which determine the dynamical properties of the models. To optimally reconstruct experimental features, it is necessary to formulate an inverse problem to extract optimally such model parameters from the experimental data. Typically this is a rather difficult problem due to the low signal-to-noise ratio in experimental brain signals. Moreover, the identification of signal features to be reconstructed by the model is not obvious in most applications. Consequently an extended analysis of the experimental data is necessary to identify the interesting data features. It is important to combine such a data analysis step with the parameter extraction procedure to achieve optimal results. Such a procedure depends on the properties of the experimental data and hence has to be developed for each application separately. Machine learning approaches that attempt to mimic the brain and its cognitive processes had a lot of success in classification problems in a last decade. These hierarchical and iterative approaches use non-linear functions, which imitate neural cell responses, to communicate messages between neighboring layers. In our team, we work towards developing polysomnography-specific classifiers that might help in linking the features of particular interest for building systems for sleep signal classification with sleep mechanisms, with the accent on memory consolidation during the Rapid Eye Movement (REM) sleep phase.

3.2. Challenges

Eventually the implementation of the models and analysis techniques achieved promises to be able to construct novel data monitor. This construction involves additional challenges and stipulates the contact to realistic environments. By virtue of the specific applications of the research, the close contact to hospitals and medical enterprises shall be established in a longer term in order to (i) gain deeper insight into the specific application of the devices and (ii) build specific devices in accordance to the actual need. Collaborations with local and national hospitals and the pharmaceutical industry already exist.

3.3. Research Directions

- From the microscopic to the mesoscopic scale:
One research direction focuses on the *relation of single neuron activity on the microscopic scale to the activity of neuronal populations*. To this end, the team investigates the stochastic dynamics of single neurons subject to external random inputs and involving random microscopic properties, such as random synaptic strengths and probability distributions of spatial locations of membrane ion channels. Such an approach yields a stochastic model of single neurons and allows the derivation of a stochastic neural population model.

This bridge between the microscopic and mesoscopic scale may be performed via two pathways. The analytical and numerical treatment of the microscopic model may be called a *bottom-up approach*,

since it leads to a population activity model based on microscopic activity. This approach allows to compare theoretical neural population activity to experimentally obtained population activity. The *top-down approach* aims at extracting signal features from experimental data gained from neural populations which give insight into the dynamics of neural populations and the underlying microscopic activity. The work on both approaches represents a well-balanced investigation of the neural system based on the systems properties.

- From the mesoscopic to the macroscopic scale:
The other research direction aims to link neural population dynamics to macroscopic activity and behaviour or, more generally, to phenomenological features. This link is more indirect but a very powerful approach to understand the brain, e.g., in the context of medical applications. Since real neural systems, such as in mammals, exhibit an interconnected network of neural populations, the team studies analytically and numerically the network dynamics of neural populations to gain deeper insight into possible phenomena, such as traveling waves or enhancement and diminution of certain neural rhythms. Electroencephalography (EEG) is a wonderful brain imaging technique to study the overall brain activity in real time non-invasively. However it is necessary to develop robust techniques based on stable features by investigating the time and frequency domains of brain signals. Two types of information are typically used in EEG signals: (i) transient events such as evoked potentials, spindles and K-complexes and (ii) the power in specific frequency bands.

ORPAILLEUR Project-Team

3. Research Program

3.1. Knowledge Discovery guided by Domain Knowledge

Keywords: knowledge discovery in databases, knowledge discovery in databases guided by domain knowledge, data mining formal concept analysis, classification, pattern mining second-order Hidden Markov Models

Knowledge discovery in databases (KDD) is aimed at discovering patterns in large databases. These patterns can then be interpreted as knowledge units to be reused in knowledge systems. From an operational point of view, the KDD process is based on three main steps: (i) selection and preparation of the data, (ii) data mining, (iii) interpretation of the discovered patterns. The KDD process –as implemented in the Orpailleur team– is based on data mining methods which are either symbolic or numerical. Symbolic methods are based on pattern mining (e.g. mining frequent itemsets, association rules, sequences...), Formal Concept Analysis (FCA [93]) and extensions of FCA such as Pattern Structures [65] and Relational Concept Analysis (RCA [101]). Numerical methods are based on probabilistic approaches such as second-order Hidden Markov Models (HMM [98]), which are well adapted to the mining of temporal and spatial data.

Domain knowledge, when available, can improve and guide the KDD process, materializing the idea of *Knowledge Discovery guided by Domain Knowledge* or KDDK. In KDDK, domain knowledge plays a role at each step of KDD: the discovered patterns can be interpreted as knowledge units and reused for problem-solving activities in knowledge systems, implementing the operational sequence “mining, interpreting (modeling), representing, and reasoning”. In this way, knowledge discovery appears as a core task in knowledge engineering, with an impact in various semantic activities, e.g. information retrieval, recommendation and ontology engineering. Moreover, it is used in application domains such as agronomy, astronomy, biology, chemistry, medicine. Accordingly, the Orpailleur team includes biologists, chemists, and a physician, making Orpailleur a very original team at Inria Nancy Grand Est.

One main operation in the research work of Orpailleur on KDDK is *classification*, which is a polymorphic process involved in modeling, mining, representing, and reasoning tasks. Classification problems can be formalized by means of a class of objects (or individuals), a class of attributes (or properties), and a binary correspondence between the two classes, indicating for each individual-property pair whether the property applies to the individual or not. The properties may be features that are present or absent, or the values of a property that have been transformed into binary variables. Formal Concept Analysis (FCA) relies on the analysis of such binary tables and may be considered as a symbolic data mining technique to be used for extracting a set of formal concepts then organized within a concept lattice [93] (concept lattices are also known as “Galois lattices” [81]).

In parallel, the search for frequent itemsets and the extraction of association rules are well-known symbolic data mining methods, related to FCA (actually searching for frequent itemsets can be understood as traversing a concept lattice). Both processes usually produce a large number of items and rules, leading to the associated problems of “mining the sets of extracted items and rules”. Some subsets of itemsets, e.g. frequent closed itemsets (FCIs), allow to find interesting subsets of association rules, e.g. informative association rules. This is why several algorithms are needed for mining data depending on specific applications [103].

3.2. Text Mining

Keywords: text mining, knowledge discovery form collection of texts, annotation, ontology engineering from texts

The objective of a text mining process is to extract useful knowledge units from large collections of texts [90]. The text mining process shows specific characteristics due to the fact that texts are complex objects written in natural language. The information in a text is expressed in an informal way, following linguistic rules, making text mining a particular task. To avoid information dispersion, a text mining process has to take into account –as much as possible– paraphrases, ambiguities, specialized vocabulary and terminology. This is why the preparation of texts for text mining is usually dependent on linguistic resources and methods.

From a KDDK perspective, text mining is aimed at extracting “interesting units” (nouns and relations) from texts with the help of domain knowledge encoded within an ontology (also useful for text annotation). Text mining is especially useful in the context of semantic web for ontology engineering. In the Orpailleur team, the focus is put on the mining of real-world texts in application domains such as biology and medicine, using mainly symbolic data mining methods, and especially Formal Concept Analysis. Accordingly, the text mining process may be involved in a loop used to enrich and to extend linguistic resources. In turn, linguistic and ontological resources can be exploited to guide a “knowledge-based text mining process”.

3.3. Knowledge Systems and Web of Data

Keywords: knowledge engineering, web of data, semantic web, ontology, description logics, classification-based reasoning, case-based reasoning, information retrieval

The web of data constitutes a good platform for experimenting ideas on knowledge engineering and knowledge discovery, in relation with the principles of semantic web. A software agent may be able to read, understand, and manipulate information on the web, if and only if the knowledge necessary for achieving those tasks is available: this is why domain knowledge and ontologies are of main importance. The knowledge representation language recommended by W3C to design ontologies and knowledge bases is OWL, which is based on description logics (DLs [79]). In OWL, knowledge units are represented by classes (or concepts) having properties (attributes) and instances. Concepts are organized within a partial order based on a subsumption relation, and the inference services are based on classification-based reasoning and case-based reasoning (CBR).

Actually, there are many interconnections between concept lattices in FCA and ontologies, e.g. the partial order underlying an ontology can be supported by a concept lattice. Moreover, a pair of implications within a concept lattice can be adapted for designing concept definitions in ontologies. Accordingly, we are interested here in two main challenges: how the web of data, as a set of potential knowledge sources (e.g. DBpedia, Wikipedia, Yago, Freebase...) can be mined for helping the design of definitions and knowledge bases and how knowledge discovery techniques can be applied for providing a better usage of the web of data (e.g. LOD classification).

Accordingly, a part of the research work in Knowledge Engineering is oriented towards knowledge discovery in the web of data, as, with the increased interest in machine processable data, more and more data is now published in RDF (Resource Description Framework) format. Particularly, we are interested in the completeness of the data and their potential to provide concept definitions in terms of necessary and sufficient conditions [1]. We have proposed a novel technique based on FCA which allows data exploration as well as the discovery of definition (bidirectional implication rules).

SEMAGRAMME Project-Team

3. Research Program

3.1. Overview

The Sémagramme project relies on deep mathematical foundations. We intend to develop models based on well-established mathematics. We seek two main advantages from this approach. On the one hand, by relying on mature theories, we have at our disposal sets of mathematical tools that we can use to study our models. On the other hand, developing various models on a common mathematical background will make them easier to integrate, and will ease the search for unifying principles.

The main mathematical domains on which we rely are formal language theory, symbolic logic, and type theory.

3.2. Formal language theory

Formal language theory studies the purely syntactic and combinatorial aspects of languages, seen as sets of strings (or possibly trees or graphs). Formal language theory has been especially fruitful for the development of parsing algorithms for context-free languages. We use it, in a similar way, to develop parsing algorithms for formalisms that go beyond context-freeness. Language theory also appears to be very useful in formally studying the expressive power and the complexity of the models we develop.

3.3. Symbolic logic

Symbolic logic (and, more particularly, proof-theory) is concerned with the study of the expressive and deductive power of formal systems. In a rule-based approach to computational linguistics, the use of symbolic logic is ubiquitous. As we previously said, at the level of syntax, several kinds of grammars (generative, categorial...) may be seen as basic deductive systems. At the level of semantics, the meaning of an utterance is captured by computing (intermediate) semantic representations that are expressed as logical forms. Finally, using symbolic logics allows one to formalize notions of inference and entailment that are needed at the level of pragmatics.

3.4. Type theory and typed λ -calculus

Among the various possible logics that may be used, Church's simply typed λ -calculus and simple theory of types (a.k.a. higher-order logic) play a central part. On the one hand, Montague semantics is based on the simply typed λ -calculus, and so is our syntax-semantics interface model. On the other hand, as shown by Gallin [43], the target logic used by Montague for expressing meanings (i.e., his intensional logic) is essentially a variant of higher-order logic featuring three atomic types (the third atomic type standing for the set of possible worlds).

SPHINX Team

3. Research Program

3.1. Control and stabilization of heterogeneous systems

Fluid-Structure Interaction Systems (FSIS) are present in many physical problems and applications. Their study require to solve several challenging mathematical problems:

- **Nonlinearity:** One has to deal with a system of nonlinear PDE such as the Navier-Stokes or the Euler systems;
- **Coupling:** The corresponding equations couple two systems of different types and the methods associated with each system need to be suitably combined to solve successfully the full problem;
- **Coordinates:** The equations for the structure are classically written with Lagrangian coordinates whereas the equations for the fluid are written with Eulerian coordinates;
- **Free boundary:** The fluid domain is moving and its motion depends on the motion of the structure. The fluid domain is thus an unknown of the problem and one has to solve a free boundary problem.

In order to control such FSIS systems, one has first to analyze the corresponding system of PDE. The oldest works on FSIS go back to the pioneering contributions of Thomson, Tait and Kirchhoff in the 19th century and Lamb in the 20th century, who considered simplified models (potential fluid or Stokes system). The first mathematical studies in the case of a viscous incompressible fluid modeled by the Navier-Stokes system and a rigid body whose dynamics is modeled by Newton's laws appeared much later [98], [90], [69], and almost all mathematical results on such FSIS have been obtained in the last twenty years.

The most studied issue concerns the well-posedness of the problem modeling a **rigid body moving into a viscous incompressible fluid**. If the fluid fills the **unbounded domain** surrounding the structure, the free boundary difficulty can be overcome by using a simple change of variables that makes the rigid body fixed. One can then use classical tools for the Navier-Stokes system and obtain the existence of weak solutions (see, for instance, [57], [58], [91]) or strong solutions for the case of a ball [95]. When the rigid body is not a ball, the additional terms due to the change of variables modify the nature of the system and only partial results are available for strong solutions [59], [45], [92]. When the fluid-solid system is confined in a **bounded domain**, the above strategy fails. Several papers have developed interesting strategies in order to obtain the existence of solutions. Since the coupling is strong, it is natural to consider a variational formulation for both the fluid and the structure equations (see [48]). One can then solve the FSIS by considering the Navier-Stokes system with a penalization term taking into account the structure ([42], [89], [53]) or using a time discretization in order to fix the rigid body during some time interval ([63]). Using an appropriate change of variables has also been used (see [62], [94]), but of course, its construction is more complex than in the case where the FSIS fills the whole space. Most of the above results only hold up to a possible contact between two structures or between a structure and the exterior boundary. If the considered configuration excludes contacts, some authors also investigated the large time behavior of this system and the existence of time periodic solutions [97], [79], [60].

Many other FSIS have been studied as well. Let us mention, for instance, **rigid bodies immersed in an incompressible perfect fluid** ([81], [66], [61]), **in a viscous compressible fluid** ([47], [35], [52], [36]), in a **viscous multipolar fluid** or in an **incompressible non-Newtonian fluid** ([54]). The case of **deformable structures** has also been considered, either for a fluid inside a moving structure (e.g. blood motion in arteries) or for a moving deformable structure immersed in a fluid (e.g. fish locomotion). Several models for the dynamics of the deformable structure exist: one can use the plate equations or the elasticity equations. The obtained coupled FSIS is a complex system and the study of its well-posedness raises several difficulties. The main one comes from the fact that we gather two systems of different nature, as the linearized problem couples a parabolic system with a hyperbolic one. Theoretical studies have been performed for approximations

of the complete system, using two strategies: adding a regularizing term in the linear elasticity equations (see [40], [35], [72]) or approximate the equations of linear elasticity by a finite dimensional system (see [49], [38]). For strong solutions, the coupling between hyperbolic-parabolic systems leads to seek solutions with high regularity. The only known results [43], [44] in this direction concern local (in time) existence of regular solutions, under strong assumptions on the regularity of the initial data. Such assumptions are not very satisfactory but seem inherent in this coupling between two systems of different natures. Another option is to consider approximate models, but so far, the available approximations are not obtained from a physical model and deriving a more realistic model is a difficult task.

In some particular important physical situations, one can also consider a simplified model. For instance, in order to study self-propelled motions of structures in a fluid, like fish locomotion, one can assume that the **deformation of the structure is prescribed and known**, whereas its displacement remains unknown ([87]). Although simplified, this model already contains many difficulties and allows starting the mathematical study of a challenging problem: understanding the locomotion mechanism of aquatic animals.

Using the above results and the corresponding tools, we aim to consider control or stabilization problems for FSIS. Some control problems have already been considered: using an interior control in the fluid region, it is possible to control locally the velocity of the fluid together with the velocity and the position of the rigid body (see [67], [37]). The strategy of control is similar to the classical method for a fluid (without solid) (see, for instance, [55]) but with the tools developed in [94]. A first result of stabilization was obtained in [83] and concerns a fluid contained in bounded cavity where a part of the boundary is modeled by a plate system. The feedback control is a force applied on the whole plate and it allows to obtain a local stabilization result around the null state.

To extend these first results of control and stabilization, we first have to make some progress in the analysis of FSIS:

- **Contact:** It is important to understand the behavior of the system when two structures are close, and in particular to understand how to deal with contact problems;
- **Deformable structures:** To handle such structures, we need to develop new ideas and techniques in order to couple two infinite-dimensional dynamics of different nature.

At the same time, we can tackle control problems for simplified models. For instance, in some regimes, the Navier-Stokes system can be replaced by the Stokes system and the Euler system by Laplace's equation

3.2. Inverse problems for heterogeneous systems

The area of inverse problems covers a large class of theoretical and practical issues which are important in many applications (see for instance the books of Isakov [68] or Kaltenbacher, Neubauer, and Scherzer [70]). Roughly speaking, an inverse problem is a problem where one attempts to recover an unknown property of a given system from its response to an external probing signal. For systems described by evolution PDE, one can be interested in the reconstruction from partial measurements of the state (initial, final or current), the inputs (a source term, for instance) or the parameters of the model (a physical coefficient for example). For stationary or periodic problems (i.e. problems where the time dependence is given), one can be interested in determining from boundary data a local heterogeneity (shape of an obstacle, value of a physical coefficient describing the medium, etc.). Such inverse problems are known to be generally ill-posed and their study leads to investigate the following questions:

- *Uniqueness.* The question here is to know whether the measurements uniquely determine the unknown quantity to be recovered. This theoretical issue is a preliminary step in the study of any inverse problem and can be a hard task.
- *Stability.* When uniqueness is ensured, the question of stability, which is closely related to sensitivity, deserves special attention. Stability estimates provides an upper bound for the parameter error given some uncertainty on data. This issue is closely related to the so-called observability inequality in systems theory.

- *Reconstruction.* Inverse problems being usually ill-posed, one needs to develop specific reconstruction algorithms which are robust with respect to noise, disturbances and discretization. A wide class of methods is based on optimization techniques.

In this project, we investigate two classes of inverse problems, which both appear in FSIS and CWS:

1. Identification for evolution PDE.

Driven by applications, the identification problem for infinite dimensional systems described by evolution PDE has known in the last three decades a fast and significant growth. The unknown to be recovered can be the (initial/final) state (e.g. state estimation problems [29], [56], [64], [93] for the design feedback controllers), an input (for instance source inverse problems [26], [39], [50]) or a parameter of the system. These -linear or non linear- problems are generally ill-posed and many regularization approaches have been developed. Among the different methods used for identification, let us mention optimization techniques ([41]), specific one dimensional techniques (like in [30]) or observer-based methods as in [77].

In the last few years, we have developed observers to solve initial data inverse problems for a class of linear infinite dimensional systems of the form $\dot{z}(t) = Az(t)$ (A denotes here the generator of a C_0 semigroup) from an output $y(t) = Cz(t)$ measured through a finite time interval. Let us recall that observers (or Luenberger observers [76]) have been introduced in automatic control theory to estimate the state of a (finite dimensional) dynamical system from the knowledge of an output (and, of course, assuming that the initial state is unknown). Roughly speaking, an observer is an auxiliary dynamical system that uses as inputs the available measurements (that is the output of the original system) that converges asymptotically (in time) towards the state of the original system. Observers are very popular in the community of automatic control and have given rise to a wide literature (for more references, see for instance the book by O'Reilly [80] and more recently the one by Trinh and Fernando [96] devoted to functional observers). The generalization of observers (also called estimators or filters in the stochastic framework) to infinite dimensional systems goes back to the seventies (see for instance Bensoussan [33] or Curtain and Zwart [46]) and the theory is definitely less developed than in the finite dimensional case. Using observers, we have proposed in [82], [65] an iterative algorithm to reconstruct initial data from partial measurements for some evolution equations, including the wave and Schrödinger systems (and more generally for skew-adjoint generators). This algorithm also provides a new method to solve source inverse problems, in the case where the source term has a specific structure (separate variables in time-space with known time dependence). We are deepening our activities in this direction by considering more general operators or more general sources and the reconstruction of coefficients for the wave equation. In connection with this last problem, we study the stability in the determination of these coefficients. To achieve this, we use geometrical optics, which is a classical albeit powerful tool to obtain quantitative stability estimates on some inverse problems with a geometrical background, see for instance [32], [31].

2. Geometric inverse problems.

We investigate some geometric inverse problems that appear naturally in many applications, like medical imaging and non destructive testing. A typical problem we have in mind is the following: given a domain Ω containing an (unknown) local heterogeneity ω , we consider the boundary value problem of the form

$$\begin{cases} Lu = 0, & (\Omega \setminus \omega) \\ u = f, & (\partial\Omega) \\ Bu = 0, & (\partial\omega) \end{cases}$$

where L is a given partial differential operator describing the physical phenomenon under consideration (typically a second order differential operator), B the (possibly unknown) operator describing the boundary condition on the boundary of the heterogeneity and f the exterior source used to probe the medium. The question is then to recover the shape of ω and/or the boundary operator B from some measurement Mu on the outer boundary $\partial\Omega$. This setting includes in particular inverse scattering problems in acoustics and electromagnetics (in this case Ω is the whole space and the data are far field measurements) and the inverse problem of detecting solids moving in a fluid. It also includes, with slight modifications, more general situations of incomplete data (i.e. measurements on part of the outer boundary) or penetrable inhomogeneities. Our approach to tackle this type of problems is based on the derivation of a series expansion of the input-to-output map of the problem (typically the Dirichlet-to-Neumann map of the problem for the Calderón problem) in terms of the size of the obstacle.

3.3. Numerical analysis and simulation of heterogenous systems

Within the team, we have developed in the last few years numerical codes for the simulation of FSIS and CWS. We plan to continue our efforts in this direction.

- In the case of FSIS, our main objective is to provide computational tools for the scientific community, essentially to solve academic problems.
- In the case of CWS, our main objective is to build softwares general enough to handle industrial problems. Our strong collaboration with Christophe Geuzaine's team in Liege (Belgium) makes this objective credible, through the combination of DDM (Domain Decomposition Methods) and parallel computing.

Below, we explain in detail the corresponding scientific program.

3.3.1. Scientific description

- **Simulation of FSIS:** In order to simulate fluid-structure systems, one has to deal with the fact that the fluid domain is moving and that the two systems for the fluid and for the structure are strongly coupled. To overcome this free boundary problem, three main families of methods are usually applied to numerically compute in an efficient way the solutions of the fluid-structure interaction systems. The first method consists in suitably displacing the mesh of the fluid domain in order to follow the displacement and the deformation of the structure. A classical method based on this idea is the A.L.E. (Arbitrary Lagrangian Eulerian) method: such a procedure allows to keep a good precision at the interface between the fluid and the structure. However, such methods are difficult to apply for large displacements (typically the motion of rigid bodies). The second family of methods consists in using a *fixed mesh* for both the fluid and the structure and to simultaneously compute the velocity field of the fluid with the displacement velocity of the structure. The presence of the structure is taken into account through the numerical scheme. There are several methods in that direction: immersed boundary method, fictitious domain method, fat boundary method, the Lagrange-Galerkin method. Finally, the third class of methods consists in transforming the set of PDEs governing the flow into a system of integral equations set on the boundary of the immersed structure. Thus, only the surface of the structure is meshed and this mesh moves along with the structure. Notice that this method can be applied only for the flow of particular fluids (ideal fluid or stationary Stokes flow).

The members of SPHINX have already worked on these three families of numerical methods for FSIS systems with rigid bodies (see e.g. [86], [71], [88], [84], [85], [78]). We plan to work on numerical methods for FSIS systems with non-rigid structures immersed into an incompressible viscous fluid. In particular, we will focus our work on the development and the analysis of numerical schemes and, on the other hand, on the efficient implementation of the corresponding numerical methods.

- **Simulation of CWS:** Solving acoustic or electromagnetic scattering problems can become a tremendously hard task in some specific situations. In the high frequency regime (i.e. for small wavelength),

acoustic (Helmholtz's equation) or electromagnetic (Maxwell's equations) scattering problems are known to be difficult to solve while being crucial for industrial applications (e.g. in aeronautics and aerospace engineering). Our particularity is to develop new numerical methods based on the hybridization of standard numerical techniques (like algebraic preconditioners, etc.) with approaches borrowed from asymptotic microlocal analysis. Most particularly, we propose to contribute to building hybrid algebraic/analytical preconditioners and quasi-optimal Domain Decomposition Methods (DDM) [34], [51],[8] for highly indefinite linear systems. Corresponding three-dimensional solvers (like for example GetDDM) will be developed and tested on realistic configurations (e.g. submarines, complete or parts of an aircraft, etc.) provided by industrial partners (Thales, Airbus). Another situation where scattering problems can be hard to solve is the one of dense multiple (acoustic, electromagnetic or elastic) scattering media. Computing waves in such media requires to take into account not only the interaction between the incident wave and the scatterers, but also the effects of the interactions between the scatterers themselves. When the number of scatterers is very large (and possibly for high frequency [28], [27]), specific deterministic or stochastic numerical methods and algorithms are needed. We propose to introduce new optimized numerical methods for solving such complex configurations. Many applications are related to this kind of problem like e.g. for osteoporosis diagnosis where quantitative ultrasound is a recent and promising technique to detect a risk of fracture. Therefore, numerical simulation of wave propagation in multiple scattering elastic medium in the high frequency regime is a very useful tool for this purpose.

TONUS Team

3. Research Program

3.1. Kinetic models for plasmas

The fundamental model for plasma physics is the coupled Vlasov-Maxwell kinetic model: the Vlasov equation describes the distribution function of particles (ions and electrons), while the Maxwell equations describe the electromagnetic field. In some applications, it may be necessary to take into account relativistic particles, which lead to consider the relativistic Vlasov equation, but generally, tokamak plasmas are supposed to be non relativistic. The particles distribution function depends on seven variables (three for space, three for velocity and one for time), which yields a huge amount of computations.

To these equations we must add several types of source terms and boundary conditions for representing the walls of the tokamak, the applied electromagnetic field that confines the plasma, fuel injection, collision effects, etc.

Tokamak plasmas possess particular features, which require developing specialized theoretical and numerical tools.

Because the magnetic field is strong, the particle trajectories have a very fast rotation around the magnetic field lines. A full resolution would require prohibitive amount of calculations. It is then necessary to develop models where the cyclotron frequency tends to infinity in order to obtain tractable calculations. The resulting model is called a gyrokinetic model. It allows us to reduce the dimensionality of the problem. Such models are implemented in GYSELA and Selalib. Those models require averaging of the acting fields during a rotation period along the trajectories of the particles. This averaging is called the gyroaverage and requires specific discretizations.

The tokamak and its magnetic fields present a very particular geometry. Some authors have proposed to return to the intrinsic geometrical versions of the Vlasov-Maxwell system in order to build better gyrokinetic models and adapted numerical schemes. This implies the use of sophisticated tools of differential geometry: differential forms, symplectic manifolds, and hamiltonian geometry.

In addition to theoretical modeling tools, it is necessary to develop numerical schemes adapted to kinetic and gyrokinetic models. Three kinds of methods are studied in TONUS: Particle-In-Cell (PIC) methods, semi-Lagrangian and fully Eulerian approaches.

3.1.1. Gyrokinetic models: theory and approximation

In most phenomena where oscillations are present, we can establish a three-model hierarchy: (i) the model parameterized by the oscillation period, (ii) the limit model and (iii) the Two-Scale model, possibly with its corrector. In a context where one wishes to simulate such a phenomenon where the oscillation period is small and where the oscillation amplitude is not small, it is important to have numerical methods based on an approximation of the Two-Scale model. If the oscillation period varies significantly over the domain of simulation, it is important to have numerical methods that approximate properly and effectively the model parameterized by the oscillation period and the Two-Scale model. Implemented Two-Scale Numerical Methods (for instance by Frénod et al. [30]) are based on the numerical approximation of the Two-Scale model. These are called of order 0. A Two-Scale Numerical Method is called of order 1 if it incorporates information from the corrector and from the equation to which this corrector is a solution. If the oscillation period varies between very small values and values of order 1, it is necessary to have new types of numerical schemes (Two-Scale Asymptotic Preserving Schemes of order 1 or TSAPS) with the property of being able to preserve the asymptotics between the model parameterized by the oscillation period and the Two-Scale model with its corrector. A first work in this direction has been initiated by Crouseilles et al. [28].

3.1.2. Semi-Lagrangian schemes

The Strasbourg team has a long and recognized experience in numerical methods of Vlasov-type equations. We are specialized in both particle and phase space solvers for the Vlasov equation: Particle-in-Cell (PIC) methods and semi-Lagrangian methods. We also have a longstanding collaboration with the CEA of Cadarache for the development of the GYSELA software for gyrokinetic tokamak plasmas.

The Vlasov and the gyrokinetic models are partial differential equations that express the transport of the distribution function in the phase space. In the original Vlasov case, the phase space is the six-dimension position-velocity space. For the gyrokinetic model, the phase space is five-dimensional because we consider only the parallel velocity in the direction of the magnetic field and the gyrokinetic angular velocity instead of three velocity components.

A few years ago, Eric Sonnendrücker and his collaborators introduce a new family of methods for solving transport equations in the phase space. This family of methods are the semi-Lagrangian methods. The principle of these methods is to solve the equation on a grid of the phase space. The grid points are transported with the flow of the transport equation for a time step and interpolated back periodically onto the initial grid. The method is then a mix of particle Lagrangian methods and eulerian methods. The characteristics can be solved forward or backward in time leading to the Forward Semi-Lagrangian (FSL) or Backward Semi-Lagrangian (BSL) schemes. Conservative schemes based on this idea can be developed and are called Conservative Semi-Lagrangian (CSL).

GYSELA is a 5D full gyrokinetic code based on a classical backward semi-Lagrangian scheme (BSL) [38] for the simulation of core turbulence that has been developed at CEA Cadarache in collaboration with our team [31]. Although GYSELA was carefully developed to be conservative at lowest order, it is not exactly conservative, which might be an issue when the simulation is under-resolved, which always happens in turbulence simulations due to the formation of vortices which roll up.

3.1.3. PIC methods

Historically PIC methods have been very popular for solving the Vlasov equations. They allow solving the equations in the phase space at a relatively low cost. The main disadvantage of the method is that, due to its random aspect, it produces an important numerical noise that has to be controlled in some way, for instance by regularizations of the particles, or by divergence correction techniques in the Maxwell solver. We have a longstanding experience in PIC methods and we started implement them in Selalib. An important aspect is to adapt the method to new multicore computers. See the work by Crestetto and Helluy [27].

3.2. Reduced kinetic models for plasmas

As already said, kinetic plasmas computer simulations are very intensive, because of the gyrokinetic turbulence. In some situations, it is possible to make assumptions on the shape of the distribution function that simplify the model. We obtain in this way a family of fluid or reduced models.

Assuming that the distribution function has a Maxwellian shape, for instance, we obtain the MagnetoHydro-Dynamic (MHD) model. It is physically valid only in some parts of the tokamak (at the edges for instance). The fluid model is generally obtained from the hypothesis that the collisions between particles are strong. Fine collision models are mainly investigated by other partners of the IPL (Inria Project Lab) FRATRES. In our approach we do not assume that the collisions are strong, but rather try to adapt the representation of the distribution function according to its shape, keeping the kinetic effects. The reduction is not necessarily a consequence of collisional effects. Indeed, even without collisions, the plasma may still relax to an equilibrium state over sufficiently long time scales (Landau damping effect). Recently, a team at the Plasma Physics Institut (IPP) in Garching has carried out a statistical analysis of the 5D distribution functions obtained from gyrokinetic tokamak simulations [32]. They discovered that the fluctuations are much higher in the space directions than in the velocity directions (see Figure 1).

This indicates that the approximation of the distribution function could require fewer data while still achieving a good representation, even in the collisionless regime.

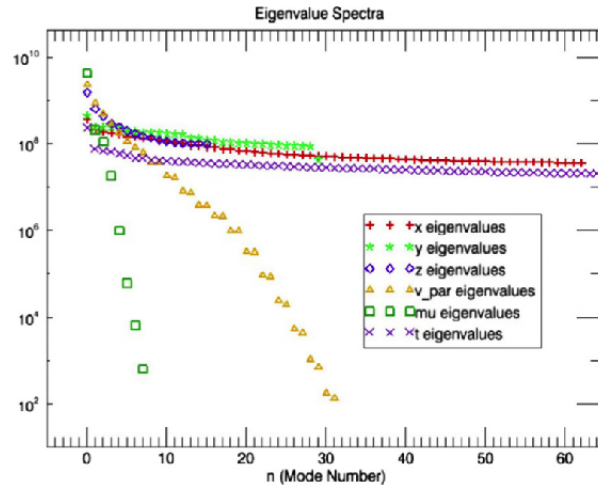


Figure 1. Space and velocity fluctuations spectra (from [32])

Our approach is different from the fluid approximation. In what follows we call this the “reduced model” approach. A reduced model is a model where the explicit dependency on the velocity variable is removed. In a more mathematical way, we consider that in some regions of the plasma, it is possible to exhibit a (preferably small) set of parameters α that allows us to describe the main properties of the plasma with a generalized “Maxwellian” M . Then

$$f(x, v, t) = M(\alpha(x, t), v).$$

In this case it is sufficient to solve for $\alpha(x, t)$. Generally, the vector α is solution of a first order hyperbolic system.

Several approaches are possible: waterbag approximations, velocity space transforms, *etc.*

3.2.1. Velocity space transformations

An experiment made in the 60’s [35] exhibits in a spectacular way the reversible nature of the Vlasov equations. When two perturbations are applied to a plasma at different times, at first the plasma seems to damp and reach an equilibrium. But the information of the perturbations is still here and “hidden” in the high frequency microscopic oscillations of the distribution function. At a later time a resonance occurs and the plasma produces an echo. The time at which the echo occurs can be computed (see Villani⁰, page 74). The fine mathematical study of this phenomenon allowed C. Villani and C. Mouhot to prove their famous result on the rigorous nonlinear Landau damping [37].

More practically, this experiment and its theoretical framework show that it is interesting to represent the distribution function by an expansion on an orthonormal basis of oscillating functions in the velocity variables. This representation allows a better control of the energy transfer between the low frequencies and the high frequencies in the velocity direction, and thus provides more relevant numerical methods. This kind of approach is studied for instance by Eliasson in [29] with the Fourier expansion.

⁰Landau damping. CEMRACS 2010 lectures. <http://smai.emath.fr/cemracs/cemracs10/PROJ/Villani-lectures.pdf>

In long time scales, filamentation phenomena result in high frequency oscillations in velocity space that numerical schemes cannot resolve. For stability purposes, most numerical schemes contain dissipation mechanisms that may affect the precision of the finest oscillations that could be resolved.

3.2.2. Adaptive modeling

Another trend in scientific computing is to optimize the computation time through adaptive modeling. This approach consists in applying the more efficient model locally, in the computational domain, according to an error indicator. In tokamak simulations, this kind of approach could be very efficient, if we are able to choose locally the best intermediate kinetic-fluid model as the computation runs. This field of research is very promising. It requires developing a clever hierarchy of models, rigorous error indicators, versatile software architecture, and algorithms adapted to new multicore computers.

3.2.3. Numerical schemes

As previously indicated, an efficient method for solving the reduced models is the Discontinuous Galerkin (DG) approach. It is possible to make it of arbitrary order. It requires limiters when it is applied to nonlinear PDEs occurring for instance in fluid mechanics. But the reduced models that we intend to write are essentially linear. The nonlinearity is concentrated in a few coupling source terms.

In addition, this method, when written in a special set of variables, called the entropy variables, has nice properties concerning the entropy dissipation of the model. It opens the door to constructing numerical schemes with good conservation properties and no entropy dissipation, as already used for other systems of PDEs [39], [25], [34], [33].

3.3. Electromagnetic solvers

A precise resolution of the electromagnetic fields is essential for proper plasma simulation. Thus it is important to use efficient solvers for the Maxwell systems and its asymptotics: Poisson equation and magnetostatics.

The proper coupling of the electromagnetic solver with the Vlasov solver is also crucial for ensuring conservation properties and stability of the simulation.

Finally plasma physics implies very different time scales. It is thus very important to develop implicit Maxwell solvers and Asymptotic Preserving (AP) schemes in order to obtain good behavior on long time scales.

3.3.1. Coupling

The coupling of the Maxwell equations to the Vlasov solver requires some precautions. The most important is to control the charge conservation errors, which are related to the divergence conditions on the electric and magnetic fields. We will generally use divergence correction tools for hyperbolic systems presented for instance in [22] (and included references).

3.3.2. Implicit solvers

As already pointed out, in a tokamak, the plasma presents several different space and time scales. It is not possible in practice to solve the initial Vlasov-Maxwell model. It is first necessary to establish asymptotic models by letting some parameters (such as the Larmor frequency or the speed of light) tend to infinity. This is the case for the electromagnetic solver and this requires implementing implicit time solvers in order to efficiently capture the stationary state, the solution of the magnetic induction equation or the Poisson equation.

TOSCA Project-Team

3. Research Program

3.1. Research Program

Most often physicists, economists, biologists and engineers need a stochastic model because they cannot describe the physical, economical, biological, etc., experiment under consideration with deterministic systems, either because of its complexity and/or its dimension or because precise measurements are impossible. Therefore, they abandon trying to get the exact description of the state of the system at future times given its initial conditions, and try instead to get a statistical description of the evolution of the system. For example, they desire to compute occurrence probabilities for critical events such as the overstepping of a given thresholds by financial losses or neuronal electrical potentials, or to compute the mean value of the time of occurrence of interesting events such as the fragmentation to a very small size of a large proportion of a given population of particles. By nature such problems lead to complex modelling issues: one has to choose appropriate stochastic models, which require a thorough knowledge of their qualitative properties, and then one has to calibrate them, which requires specific statistical methods to face the lack of data or the inaccuracy of these data. In addition, having chosen a family of models and computed the desired statistics, one has to evaluate the sensitivity of the results to the unavoidable model specifications. The TOSCA team, in collaboration with specialists of the relevant fields, develops theoretical studies of stochastic models, calibration procedures, and sensitivity analysis methods.

In view of the complexity of the experiments, and thus of the stochastic models, one cannot expect to use closed form solutions of simple equations in order to compute the desired statistics. Often one even has no other representation than the probabilistic definition (e.g., this is the case when one is interested in the quantiles of the probability law of the possible losses of financial portfolios). Consequently the practitioners need Monte Carlo methods combined with simulations of stochastic models. As the models cannot be simulated exactly, they also need approximation methods which can be efficiently used on computers. The TOSCA team develops mathematical studies and numerical experiments in order to determine the global accuracy and the global efficiency of such algorithms.

The simulation of stochastic processes is not motivated by stochastic models only. The stochastic differential calculus allows one to represent solutions of certain deterministic partial differential equations in terms of probability distributions of functionals of appropriate stochastic processes. For example, elliptic and parabolic linear equations are related to classical stochastic differential equations (SDEs), whereas nonlinear equations such as the Burgers and the Navier–Stokes equations are related to McKean stochastic differential equations describing the asymptotic behavior of stochastic particle systems. In view of such probabilistic representations one can get numerical approximations by using discretization methods of the stochastic differential systems under consideration. These methods may be more efficient than deterministic methods when the space dimension of the PDE is large or when the viscosity is small. The TOSCA team develops new probabilistic representations in order to propose probabilistic numerical methods for equations such as conservation law equations, kinetic equations, and nonlinear Fokker–Planck equations.

VEGAS Project-Team (section vide)

VERIDIS Project-Team

3. Research Program

3.1. Automated and Interactive Theorem Proving

The VeriDis team gathers experts in techniques and tools for automatic deduction and interactive theorem proving, and specialists in methods and formalisms designed for the development of trustworthy concurrent and distributed systems and algorithms. Our common objective is twofold: first, we wish to advance the state of the art in automated and interactive theorem proving, and their combinations. Second, we work on making the resulting technology available for the computer-aided verification of distributed systems and protocols. In particular, our techniques and tools are intended to support sound methods for the development of trustworthy distributed systems that scale to algorithms relevant for practical applications.

VeriDis members from Saarbrücken are developing SPASS [10], one of the leading automated theorem provers for first-order logic based on the superposition calculus [50]. The group also studies general frameworks for the combination of theories such as the locality principle [70] and automated reasoning mechanisms these induce. Finally, members of the group design effective quantifier elimination methods and decision procedures for algebraic theories, supported by their efficient implementation in the Redlog system [4].

In a complementary approach to automated deduction, VeriDis members from Nancy work on techniques for integrating reasoners for specific theories. They develop veriT[1], an SMT (Satisfiability Modulo Theories [52]) solver that combines decision procedures for different fragments of first-order logic and that integrates an automatic theorem prover for full first-order logic. The veriT solver is designed to produce detailed proofs; this makes it particularly suitable as a component of a robust cooperation of deduction tools.

An important objective of this line of work is the integration of theories in automated deduction. Typical theories of interest, including fragments of arithmetic, are not expressible in first-order logic. We therefore explore efficient, modular techniques for integrating semantic and syntactic reasoning methods, develop novel combination results and techniques for quantifier instantiation. These problems are addressed from both sides, e.g. by embedding a decision procedure into the superposition framework or by allowing an SMT solver to accept axiomatizations for plug-in theories. We also develop specific decision procedures for theories such as non-linear real arithmetic that are important when reasoning about certain classes of (e.g., real-time) systems but that also have interesting applications beyond verification.

We rely on interactive theorem provers for reasoning about specifications at a high level of abstraction when fully automatic verification is not (yet) feasible. An interactive proof platform should help verification engineers lay out the proof structure at a sufficiently high level of abstraction; powerful automatic plug-ins should then discharge the resulting proof steps. Members of VeriDis have ample experience in the specification and subsequent machine-assisted, interactive verification of algorithms. In particular, we participate in a project at the joint MSR-Inria Centre in Saclay on the development of methods and tools for the formal proof of TLA⁺ [64] specifications. Our prover relies on a declarative proof language, and calls upon several automatic backends [3]. Trust in the correctness of the overall proof can be ensured when the backends provide justifications that can be checked by the trusted kernel of a proof assistant. During the development of a proof, most obligations that are passed to the prover actually fail – for example, because necessary information is not present in the context or because the invariant is too weak, and we are interested in explaining failed proof attempts to the user, in particular through the construction of counter-models.

3.2. Formal Methods for Developing Algorithms and Systems

Powerful theorem provers are not used in isolation, but they support the application of sound methodologies for modeling and verifying systems. In this respect, members of VeriDis have gained expertise and recognition in making contributions to formal methods for concurrent and distributed algorithms and systems [2], [9], and

in applying them to concrete use cases. In particular, the concept of *refinement* [49], [51], [66] in state-based modeling formalisms is central to our approach because it allows us to present a rational (re)construction of system development. An important goal in designing such methods is to establish precise proof obligations many of which can be discharged by automatic tools. This requires taking into account specific characteristics of certain classes of systems and tailoring the model to concrete computational models. Our research in this area is supported by carrying out case studies for academic and industrial developments. This activity benefits from and influences the development of our proof tools.

In this line of work, we investigate specific development and verification patterns for particular classes of algorithms, in order to reduce the work associated with verifying specific algorithms. We are also interested in applications of formal methods and their associated tools to the development of systems that underlie specific certification requirements in the sense of, e.g., Common Criteria. Finally, we are interested in the adaptation of model checking techniques for verifying actual distributed programs, rather than high-level models.

Today, the formal verification of a new algorithm is typically the subject of a PhD thesis, if it is addressed at all. This situation is not sustainable given the move towards more and more parallelism in mainstream systems: algorithm developers and system designers must be able to productively use verification tools for validating their algorithms and implementations. On a high level, the goal of VeriDis is to make formal verification standard practice for the development of distributed algorithms and systems, just as symbolic model checking has become commonplace in the development of embedded systems and as security analysis for cryptographic protocols is becoming standard practice today. Although the fundamental problems in distributed programming are well-known, they pose new challenges in the context of modern system paradigms, including ad-hoc and overlay networks or peer-to-peer systems, and they must be integrated for concrete applications.