RESEARCH CENTER

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BACCHUS Team

3. Research Program

3.1. Numerical schemes for fluid mechanics

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A large number of engineering problems involve fluid mechanics. They may involve the coupling of one or more physical models. An example is provided by aeroelastic problems, which have been studied in details by other Inria teams. Another example is given by flows in pipelines where the fluid (a mixture of air–water–gas) does not have well-known physical properties, and there are even more exotic situations. In some occasions, one needs specific numerical tools to take into account *e.g.* a fluids' exotic equation of state, or a the influence of small flow scales in a macro-/meso-scopic flow model, etc. Efficient schemes are needed in unsteady flows where the amount of required computational resources becomes huge. Another situation where specific tools are needed is when one is interested in very specific physical quantities, such as *e.g.* the lift and drag of an airfoil, or the boundary of the area flooded by a Tsunami.

In these situations, commercial tools can only provide a crude answer. These codes, while allowing users to simulate a lot of different flow types, and "always" providing an answer, often give results of poor quality. This is mainly due to their general purpose character, and on the fact that the numerical technology implemented in these codes is not the most recent. To give a few examples, consider the noise generated by wake vortices in supersonic flows (external aerodynamics/aeroacoustics), or the direct simulation of a 3D compressible mixing layer in a complex geometry (as in combustion chambers). Up to our knowledge, due to the very different temporal and physical scales that need to be captured, a direct simulation of these phenomena is not in the reach of the most recent technologies because the numerical resources required are currently unavailable. *We need to invent specific algorithms for this purpose.*

Our goal is to develop more accurate and more efficient schemes that can adapt to modern computer architectures, and allow the efficient simulation of complex real life flows.

We develop a class of numerical schemes, known in literature as Residual Distribution schemes, *specifically tailored to unstructured and hybrid meshes*. They have the most possible compact stencil that is compatible with the expected order of accuracy. This *accuracy is at least of second order, and it can go up to any order of accuracy, even though fourth order is considered for practical applications.* Since the stencil is compact, the implementation on parallel machines becomes simple. These schemes are very flexible in nature, which is so far one of the most important advantage over other techniques. This feature has allowed us to adapt the schemes to the requirements of different physical situations (*e.g.* different formulations allow either en efficient explicit time advancement for problems involving small time-scales, or a fully implicit space-time variant which is unconditionally stable and allows to handle stiff problems where only the large time scales are relevant). This flexibility has also enabled to devise a variant using the same data structure of the popular Discontinuous Galerkin schemes, which are also part of our scientific focus.

The compactness of the second order version of the schemes enables us to use efficiently the high performance parallel linear algebra tools developed by the team. However, the high order versions of these schemes, which are under development, require modifications to these tools taking into account the nature of the data structure used to reach higher orders of accuracy. This leads to new scientific problems at the border between numerical analysis and computer science. In parallel to these fundamental aspects, we also work on adapting more classical numerical tools to complex physical problems such as those encountered in interface flows, turbulent or multiphase flows, geophysical flows, and material science. A particular attention has been devoted to the implementation of complex thermodynamic models permitting to simulate several classes of fluids and to take into account real-gas effects and some exotic phenomenon, such as rarefaction shock waves.

Within these applications, a strong effort has been made in developing more predictive tools for both multiphase compressible flows and non-hydrostatic free surface flows.

Concerning multiphase flows, several advancements have been performed, i.e. considering a more complete systems of equations including viscosity, working on the thermodynamic modelling of complex fluids, and developing stochastic methods for uncertainty quantification in compressible flows. Concerning depth averaged free surface flow modelling, on one hand we have shown the advantages of the use of the compact schemes we develop for hydrostatic shallow water models. On the other, we have shown ho to extend our approach to non-hydrostatic Boussinesq modelling, including wave dispersion, and wave breaking effects.
We expect to be able to demonstrate the potential of our developments on applications ranging from the the reproduction of the complex multidimensional interactions between tidal waves and estuaries, to the unsteady aerodynamics and aeroacoustics associated to both external and internal compressible flows, and the behaviour of complex materials. This will be achieved by means of a multi-disciplinary effort involving our research on residual discretizations schemes, the parallel advances in algebraic solvers and partitioners, and the strong interactions with specialists in computer science, scientific computing, physics, mechanics, and mathematical modeling.
Concerning the software platforms, our research in numerical algorithms has led to the development of the `RealfluiDS` platform which is described in section 4.3 , and to the `SLOWS` (Shallow-water fLOWS) code for free surface flows, described in sections 4.10 . Simultaneously, we have contributed to the advancement of the new, object oriented, parallel finite elements library `AeroSol`, described in section 4.1 , which is destined to replace the existing codes and become the team's CFD kernel. Concerning uncertainty quantification and robust optimization, we are developing the platform `RobUQ`.

New software developments are under way in the field of complex materials modeling and multiphase flows with heat and mass transfer. Concerning the materials modelling, these developments are performed in the code in the solver `COCA` (CodeOxydationCompositesAutocicatrisants) for the simulation of the self-healing process in composite materials. These developments will be described in section 4.2 . Concerning the numerical simulation of multiphase flows, we have developed the code `sDEM`, which is one of rare code, permitting to simulate metastable states with a complex thermodynamics and considering uncertainty quantification techniques.
Funding and external collaborations. This work is supported by several sources including the last of the `ADDECCO` ERC grant, the FP7 STORM, the ANR `UFO` and the PIA project `TANDEM`. Important contributions to these activities are given by our external collaborators, and in particular R. Abgrall (Universität Zürich), P. Bonneton (UMR EPOC Bordeaux), G. Vignoles (LCTS lab Bordeaux), and D. De Santis (via the associated team `AQUARIUS`).

3.2. Numerical schemes for Uncertainty quantification and robust optimization

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Another topic of interest is the quantification of uncertainties in non linear problems. In many applications, the physical model is not known accurately. The typical example is that of turbulence models in aeronautics. These models all depend on a number of parameters which can radically change the output of the simulation. Being impossible to lump the large number of temporal and spatial scales of a turbulent flow in a few model parameters, these values are often calibrated to quantitatively reproduce a certain range of effects observed experimentally. A similar situation is encountered in many applications such as real gas or multiphase flows, where the equation of state form suffer from uncertainties, and free surface flows with sediment transport, where often both the hydrodynamic model and the sediment transport model depend on several parameters, and my have more than one formal expression.

This type of uncertainty, called *epistemic*, is associated with a lack of knowledge and could be reduced by further experiments and investigation. Instead, another type of uncertainty, called *aleatory*, is related to the intrinsec aleatory quality of a physical measure and can not be reduced. The dependency of the numerical simulation from these uncertainties can be studied by propagation of chaos techniques such as those developed during the recent years via polynomial chaos techniques. Different implementations exists, depending whether the method is intrusive or not. The accuracy of these methods is still a matter of research, as well how they can handle an as large as possible number of uncertainties or their versatility with respect to the structure of the random variable pdfs.

Our objective is to develop some non-intrusive and semi-intrusive methods, trying to define an unified framework for obtained a reliable and accurate numerical solution at a moderate computational cost. This work have produced a large number of publications on peer-reviewed journal. Concerning the class of intrusive methods, we are developing an unified scheme in the coupled physical/stochastic space based on a multi-resolution framework. Here, the idea is to build a framework for being capable to refine a discontinuity in both stochastic and deterministic mesh. We are extending this class of methods to complex models in CFD, such as in multiphase flows. Concerning the non-intrusive methods, we are working on several methods for treating the following problems : handling a large number of uncertainties, treating high-order statistical decomposition (variance, skewness and kurtosis), and solving efficiently inverse problems.

We have used these methods to several ends: either to have highly accurate quantitative reconstruction of a simulation output's variation over a complex space of parameter variations to study a given model (uncertainty propagation), or as a means of comparing different model's variability to certain parameters thus assessing their robustness (model robustness), or as a tool to compare different numerical implementation (schemes and codes) of a similar model to assess simultaneously the robustness of the numerics and the universality of the trends of the statistics and of the sensitivity measures (robust cross-validation). Moreover, we rebuild statistically some input parameters relying on some experimental measures of the output, thus solving an inverse problem.

The developed methods and tools have been applied to several applications of interest : real-gas effects, multi-phase flows, cavitation, aerospace applications and geophysical flows.

Concerning robust optimization, we focus on problems with high dimensional representation of stochastic inputs, that can be computationally prohibitive. In fact, for a robust design, statistics of the fitness functions are also important, then uncertainty quantification (UQ) becomes the predom- inant issue to handle if a large number of uncertainties is taken into account. Several methods are proposed in literature to consider high dimension stochastic problem but their accuracy on realistic problems where highly non-linear effects could exist is not proven at all. We developed several efficient global strategies for robust optimization: the first class of method is based on the extension of simplex stochastic collocation to the optimization space, the second one consists in hybrid strategies using ANOVA decomposition.

These developments and computations are performed in the platform `RobUQ`, which includes the most part of methods developed in the Team.
Funding and external collaborations. This part of our activities is supported by the ANR-MN project `UFO`, and the associated team `AQUARIUS`. It benefits from the collaborations with external members, and in particular R. Abgrall (Universität Zürich), and of the members of the associated team.

3.3. Meshes and scalable discrete data structures

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3.3.1. Dynamic mesh adaptation and partitioning

Many simulations which model the evolution of a given phenomenon along with time (turbulence and unsteady flows, for instance) need to re-mesh some portions of the problem graph in order to capture more accurately the properties of the phenomenon in areas of interest. This re-meshing is performed according to criteria which are closely linked to the undergoing computation and can involve large mesh modifications: while elements are created in critical areas, some may be merged in areas where the phenomenon is no longer critical. To alleviate the cost of this re-meshing phase, we have started looking into time dependent continuous mesh deformation techniques. These may allow some degree of adaptation between two re-meshing phases, which in theory may be less frequent, and more local.

When working in parallel, re-meshing introduces additional problems. In particular, splitting an element which is located on the frontier between several processors is not an easy task, because deciding when splitting some element, and defining the direction along which to split it so as to preserve numerical stability most, require shared knowledge which is not available in distributed memory architectures. Ad-hoc data structures and algorithms have to be devised so as to achieve these goals without resorting to extra communication and synchronization which would impact the running speed of the simulation.

Most of the works on parallel mesh adaptation attempt to parallelize in some way all the mesh operations: edge swap, edge split, point insertion, etc. It implies deep modifications in the (re)mesher and often leads to bad performance in term of CPU time. An other work [54] proposes to base the parallel re-meshing on existing mesher and load balancing to be able to modify the elements located on the frontier between several processors.

In addition, the preservation of load balance in the re-meshed simulation requires dynamic redistribution of mesh data across processing elements. Several dynamic repartitioning methods have been proposed in the literature [55], [53], which rely on diffusion-like algorithms and the solving of flow problems to minimize the amount of data to be exchanged between processors. However, integrating such algorithms into a global framework for handling adaptive meshes in parallel has yet to be done.

The path that we are following bases on the decomposition of the areas to remesh into balls that can be processed concurrently, each by a sequential remesher. It requires to devise scalable algorithms for building such boules, scheduling them on as many processors as possible, reconstructing the remeshed mesh and redistributing its data.
Funding and external collaborations. Most of this research has started within the context of the PhD of Cédric Lachat, funded by a CORDI grant of EPI `PUMAS` and was continued thanks to a funding by ADT grant `El Gaucho` that completed this year. The work on adaptation by continuous deformation has started with the PhD of L. Arpaia and benefits of the funding of the PIA project `TANDEM`.

3.3.2. Graph partitioning and static mapping

Unlike their predecessors of two decades ago, today's very large parallel architectures can no longer implement a uniform memory model. They are based on a hierarchical structure, in which cores are assembled into chips, chips are assembled into boards, boards are assembled into cabinets and cabinets are interconnected through high speed, low latency communication networks. On these systems, communication is non uniform: communicating with cores located on the same chip is cheaper than with cores on other boards, and much cheaper than with cores located in other cabinets. The advent of these massively parallel, non uniform machines impacts the design of the software to be executed on them, both for applications and for service tools. It is in particular the case for the software whose task is to balance workload across the cores of these architectures.

A common method for task allocation is to use graph partitioning tools. The elementary computations to perform are represented by vertices and their dependencies by edges linking two vertices that need to share some piece of data. Finding good solutions to the workload distribution problem amounts to computing partitions with small vertex or edge cuts and that balance evenly the weights of the graph parts. Yet, computing efficient partitions for non uniform architectures requires to take into account the topology of the target architecture. When processes are assumed to coexist simultaneously for all the duration of the program, this generalized optimization problem is called mapping. In this problem, the communication cost function to minimize incorporates architecture-dependent, locality improving terms, such as the dilation of each edge (that is, by how much it is "stretched" across the graph representing the target architecture), which is sometimes also expressed as some “hop metric”. A mapping is called static if it is computed prior to the execution of the program and is never modified at run-time.

The sequential `Scotch` tool being developed within the `BACCHUS` team (see Section 4.9) was able to perform static mapping since its first version, in 1994, but this feature was not widely known nor used by the community. With the increasing need to map very large problem graphs onto very large and strongly non uniform parallel machines, there is an increasing demand for parallel static mapping tools. Since, in the context of dynamic repartitioning, parallel mapping software will have to run on their target architectures, parallel mapping and remapping algorithms suitable for efficient execution on such heterogeneous architectures have to be investigated. This leads to solve three interwoven challenges:

- scalability: such algorithms must be able to map graphs of more than a billion vertices onto target architectures comprising millions of cores;
- heterogeneity: not only do these algorithms must take into account the topology of the target architecture they map graphs onto, but they also have themselves to run efficiently on these very architectures;
- asynchronicity: most parallel partitioning algorithms use collective communication primitives, that is, some form of heavy synchronization. With the advent of machines having several millions of cores, and in spite of the continuous improvement of communication subsystems, the demand for more asynchronicity in parallel algorithms is likely to increase.

This year, our work mostly concerned the tighter integration of `Scotch` with `PaMPA`. In particular, the routines for partitioning with fixed vertices, which are mandatory in `PaMPA` to balance remeshing workload across processing elements that already contain some mesh data, have been redesigned almost from scratch.

CAGIRE Team

3. Research Program

3.1. Computational fluid mechanics: resolving versus modelling small scales of turbulence

A typical continuous solution of the Navier Stokes equations is governed by a spectrum of time and space scales. The broadness of that spectrum is directly controlled by the Reynolds number defined as the ratio between the inertial forces and the viscous forces. This number is quite helpful to determine if the flow is turbulent or not. In the former case, it indicates the range of scales of fluctuations that are present in the flow under study. Typically, for instance for the velocity field, the ratio between the largest scale (the integral length scale) to the smallest one (Kolmogorov scale) scales as $Re^{3/4}$ per dimension. In addition, for internal flows, the viscous effects near the solid walls yield a scaling proportional to Re per dimension. The smallest scales may have a certain effect on the largest ones which implies that an accurate framework for the modelling and the computation of such turbulent flows must take into account all these scales of time and space fluctuations. This can be achieved either by solving directly the Navier-Stokes (NS) equations (Direct numerical simulations or DNS) or by first applying to them a filtering operation either in time or space. In the latter cases, the closure of the new terms that appear in the filtered equations due to the presence of the non-linear terms implies the recourse to a turbulence model before discretizing and then solving the set of resulting governing equations. Among these different methodologies, the Reynolds averaged Navier-Stokes (RANS) approach yields a system of equations aimed at describing the mean flow properties. The term mean is referring to an ensemble average which is equivalent to a time average only when the flow is statistically stationnary. In that case, the turbulence model aims at expressing the Reynolds stresses either through the solution of dedicated transport equations (second order modelling) or via the recourse to the concept of turbulent viscosity used to write and ad-hoc relation (linear or not) between the Reynolds stress and the mean velocity gradient tensor. If the filtering operation involves a convolution with a filter function in space of width δ, this corresponds to the large-eddy simulation (LES) approach. The structures of size below δ are filtered out while the bigger structures are directly resolved. The resulting set of filtered equations is again not closed and calls for a model aimed at providing a suitable expression for the subgrid scale stress tensor.

From a computational point of view, the RANS approach is the less demanding, which explains why historically it has been the workhorse in both the academic and the industrial sectors. Although it has permitted quite a substantive progress in the understanding of various phenomena such as turbulent combustion or heat transfer, its inability to provide a time-dependent information has led to promote in the last decade the recourse to either LES or DNS as well as hybrid methods that combine RANS and LES. By simulating the large scale structures while modelling the smallest ones supposed to be more isotropic, the LES, alone or combined with the most adanced RANS models such as the EB-RSM model [4] proved to be quite a step through that permits to fully take advantage of the increasing power of computers to study complex flow configurations. In the same time, DNS was progressively applied to geometries of increasing complexity (channel flows, jets, turbulent premixed flames), and proved to be a formidable tool that permits **(i)** to improve our knowledge of turbulent flows and **(ii)** to test (i.e. validate or invalidate) and improve the numerous modelling hypotheses inherently associated to the RANS and LES approaches. From a numerical point of view, if the steady nature of the RANS equations allows to perform iterative convergence on finer and finer meshes, this is no longer possible for LES or DNS which are time-dependent. It is therefore necessary to develop high accuracy schemes in such frameworks. Considering that the Reynolds number in an engine combustion chamber is significantly larger than 10000, a direct numerical simulation of the whole flow domain is not conceivable on a routine basis but the simulation of generic flows which feature some of the phenomena present in a combustion chamber is accessible considering the recent progresses in High Performance Computing (HPC).

3.2. Computational fluid mechanics: numerical methods

All the methods we describe are mesh-based methods: the computational domain is divided into *cells*, that have an elementary shape: triangle and quadrangle in two dimensions, and tetrahedra, hexahedra, pyramids, and prism in three dimensions. If the cells are only regular hexahedra, the mesh is said to be *structured*. Otherwise, it is said to be unstructured. If the mesh is composed of more than one sort of elementary shape, the mesh is said to be *hybrid*.

The basic numerical model for the computation of internal flows is based on the Navier-Stokes equations. For fifty years, many sorts of numerical approximation have been tried for this sort of system: finite differences, finite volumes, and finite elements.

The finite differences have met a great success for some equations, but for the approximation of fluid mechanics, they suffer from two drawbacks. First, structured meshes must be used. This drawback can be very limiting in the context of internal aerodynamics, in which the geometries can be very complex. The other problem is that finite difference schemes do not include any upwinding process, which is essential for convection dominated flows.

The finite volumes methods have imposed themselves in the last thirty years in the context of aerodynamic. They intrinsically contain an upwinding mechanism, so that they are naturally stable for linear as much as for nonlinear convective flows. The extension to diffusive flows has been done in [18]. Whereas the extension to second order with the MUSCL method is widely spread, the extension to higher order has always been a strong drawback of finite volumes methods. For such an extension, reconstruction methods have been developed (ENO, WENO). Nevertheless, these methods need to use a stencil that increases quickly with the order, which induces problems for the parallelisation and the efficiency of the implementation. Another natural extension of finite volume methods are the so-called discontinuous Galerkin methods. These methods are based on the Galerkin' idea of projecting the weak formulation of the equations on a finite dimensional space. But on the contrary to the conforming finite elements method, the approximation space is composed of functions that are continuous (typically: polynomials) inside each cell, but that are discontinuous on the sides. The discontinuous Galerkin methods are currently very popular, because they can be used with many sort of partial differential equations. Moreover, the fact that the approximation is discontinuous allows to use modern mesh adaptation (hanging nodes, which appear in non conforming mesh adaptation), and adaptive order, in which the high order is used only where the solution is smooth.

Discontinuous Galerkin methods where introduced by Reed and Hill [39] and first studied by Lesaint and Raviart [32]. The extension to the Euler system with explicit time integration was mainly led by Shu, Cockburn and their collaborators. The steps of time integration and slope limiting were similar to high order ENO schemes, whereas specific constraints given by the finite elements nature of the scheme were progressively solved, for scalar conservation laws [22], [21], one dimensional systems [20], multidimensional scalar conservation laws [19], and multidimensional systems [23]. For the same system, we can also cite the work of [25], [30], which is slightly different: the stabilisation is made by adding a nonlinear stabilisation term, and the time integration is implicit. Then, the extension to the compressible Navier-Stokes system was made by Bassi and Rebay [17], first by a mixed type finite element method, and then simplified by means of lifting operators. The extension to the $k-\omega$ RANS system was made in [16]. Another type of discontinuous Galerkin method for Navier Stokes is the so-called Symmetric Interior Penalty (SIP) method. It is used for example by Hartmann and Houston [28]. The symmetric nature of the discretization is particularly well suited with mesh adaptation by means of the adjoint equation resolution [29]. Last, we note that the discontinuous Galerkin method was already successfully tested in [24] at Direct Numerical Simulation scale for very moderate Reynolds, and also by the Munz's team in Stuttgart [33], with local time stepping.

For concluding this section, there already exist numerical schemes based on the discontinuous Galerkin method which proved to be efficient for computing compressible viscous flows. Nevertheless, there remain things to be improved, which include: efficient shock capturing term methods for supersonic flows, high order discretization of curved boundaries, or low Mach behaviour of these schemes. Another drawback of the discontinuous Galerkin methods is that they are very computationally costly, due to the accurate representation of the solution. Accordingly, a particular care must be taken on the implementation for being efficient.

3.3. Flow analysis and CFD assessment: experimental aspects

The capability of producing in-situ experimental data is another originality of our project. By carefully controlling the flow configuration and the type of data we are measuring, we are in situation of assessing in depth the quality of our simulations results over the complete spectrum of possible approaches ranging from DNS, RANS and Hybrid RANS-LES models that the team is developing or LES.

The flow configuration we have chosen is that of a jet in cross-flow since it features large scale coherent structures, flow separation, turbulence and wall-flow interaction.

A great deal of experiments has been devoted to the study of jet in crossflow configurations. They essentially differ one from each other by the hole shape (cylindrical or shaped), the hole axis inclination, the way by which the hole is fed, the characteristics of the crossflow and the jet (turbulent or not, isothermal or not), the number of holes considered and last but not least the techniques used to investigate the flow. A good starting point to assess the diversity of the studies carried out is given by [34]. For inclined cylindrical holes, the experimental database produced by Gustafsson and Johansson [0] represents a sound reference base and for normal injection, the work by [40] served as reference for LES simulations [38]. For shaped holes, the studies are less numerous and are aimed at assessing the influence of the hole shape on various flow properties such as the heat transfer at the wall [31]. In 2007, Most [35] developed at UPPA a test facility for studying jet in crossflow issued from shaped holes. The hole shape was chosen as a 12.5 scale of the holes (i.e. at scale 1) drilled by laser in a combustion chamber. His preliminary 2-component PIV results have been used to test RANS simulations [36] and LES [37]. Later, in the framework of the KIAI FP7 European programme, Florenciano [26] upgraded the rig by implementing an acoustic forcing device of the crossflow stream and by performing phase-locked PIV measurements that were used to test the accuracy of LES results. Thus, this test facility is extensively used in the framework of the present project to investigate a 1-hole cylindrical inclined jet interacting with a turbulent crossflow. PIV and LDV metrology are the workhorses as far as metrology is concerned.

[0] Slanted jet

DEFI Project-Team

3. Research Program

3.1. Research Program

The research activity of our team is dedicated to the design, analysis and implementation of efficient numerical methods to solve inverse and shape/topological optimization problems in connection with wave imaging, structural design, non-destructive testing and medical imaging modalities. We are particularly interested in the development of fast methods that are suited for real-time applications and/or large scale problems. These goals require to work on both the physical and the mathematical models involved and indeed a solid expertise in related numerical algorithms.

This section intends to give a general overview of our research interests and themes. We choose to present them through the specific academic example of inverse scattering problems (from inhomogeneities), which is representative of foreseen developments on both inversion and (topological) optimization methods. The practical problem would be to identify an inclusion from measurements of diffracted waves that result from the interaction of the sought inclusion with some (incident) waves sent into the probed medium. Typical applications include biomedical imaging where using micro-waves one would like to probe the presence of pathological cells, or imaging of urban infrastructures where using ground penetrating radars (GPR) one is interested in finding the location of buried facilities such as pipelines or waste deposits. This kind of applications requires in particular fast and reliable algorithms.

By “imaging” we shall refer to the inverse problem where the concern is only the location and the shape of the inclusion, while “identification” may also indicate getting informations on the inclusion physical parameters.

Both problems (imaging and identification) are non linear and ill-posed (lack of stability with respect to measurements errors if some careful constrains are not added). Moreover, the unique determination of the geometry or the coefficients is not guaranteed in general if sufficient measurements are not available. As an example, in the case of anisotropic inclusions, one can show that an appropriate set of data uniquely determine the geometry but not the material properties.

These theoretical considerations (uniqueness, stability) are not only important in understanding the mathematical properties of the inverse problem, but also guide the choice of appropriate numerical strategies (which information can be stably reconstructed) and also the design of appropriate regularization techniques. Moreover, uniqueness proofs are in general constructive proofs, i.e. they implicitly contain a numerical algorithm to solve the inverse problem, hence their importance for practical applications. The sampling methods introduced below are one example of such algorithms.

A large part of our research activity is dedicated to numerical methods applied to the first type of inverse problems, where only the geometrical information is sought. In its general setting the inverse problem is very challenging and no method can provide a universal satisfactory solution to it (regarding the balance cost-precision-stability). This is why in the majority of the practically employed algorithms, some simplification of the underlying mathematical model is used, according to the specific configuration of the imaging experiment. The most popular ones are geometric optics (the Kirchhoff approximation) for high frequencies and weak scattering (the Born approximation) for small contrasts or small obstacles. They actually give full satisfaction for a wide range of applications as attested by the large success of existing imaging devices (radar, sonar, ultrasound, X-ray tomography, etc.), that rely on one of these approximations.

Generally speaking, the used simplifications result in a linearization of the inverse problem and therefore are usually valid only if the latter is weakly non-linear. The development of these simplified models and the improvement of their efficiency is still a very active research area. With that perspective we are particularly interested in deriving and studying higher order asymptotic models associated with small geometrical parameters such as: small obstacles, thin coatings, wires, periodic media, ... Higher order models usually introduce some non linearity in the inverse problem, but are in principle easier to handle from the numerical point of view than in the case of the exact model.

A larger part of our research activity is dedicated to algorithms that avoid the use of such approximations and that are efficient where classical approaches fail: i.e. roughly speaking when the non linearity of the inverse problem is sufficiently strong. This type of configuration is motivated by the applications mentioned below, and occurs as soon as the geometry of the unknown media generates non negligible multiple scattering effects (multiply-connected and closely spaces obstacles) or when the used frequency is in the so-called resonant region (wave-length comparable to the size of the sought medium). It is therefore much more difficult to deal with and requires new approaches. Our ideas to tackle this problem will be motivated and inspired by recent advances in shape and topological optimization methods and also the introduction of novel classes of imaging algorithms, so-called sampling methods.

The sampling methods are fast imaging solvers adapted to multi-static data (multiple receiver-transmitter pairs) at a fixed frequency. Even if they do not use any linearization the forward model, they rely on computing the solutions to a set of linear problems of small size, that can be performed in a completely parallel procedure. Our team has already a solid expertise in these methods applied to electromagnetic 3-D problems. The success of such approaches was their ability to provide a relatively quick algorithm for solving 3-D problems without any need for a priori knowledge on the physical parameters of the targets. These algorithms solve only the imaging problem, in the sense that only the geometrical information is provided.

Despite the large efforts already spent in the development of this type of methods, either from the algorithmic point of view or the theoretical one, numerous questions are still open. These attractive new algorithms also suffer from the lack of experimental validations, due to their relatively recent introduction. We also would like to invest on this side by developing collaborations with engineering research groups that have experimental facilities. From the practical point of view, the most potential limitation of sampling methods would be the need of a large amount of data to achieve a reasonable accuracy. On the other hand, optimization methods do not suffer from this constrain but they require good initial guess to ensure convergence and reduce the number of iterations. Therefore it seems natural to try to combine the two class of methods in order to calibrate the balance between cost and precision.

Among various shape optimization methods, the Level Set method seems to be particularly suited for such a coupling. First, because it shares similar mechanism as sampling methods: the geometry is captured as a level set of an “indicator function” computed on a cartesian grid. Second, because the two methods do not require any a priori knowledge on the topology of the sought geometry. Beyond the choice of a particular method, the main question would be to define in which way the coupling can be achieved. Obvious strategies consist in using one method to pre-process (initialization) or post-process (find the level set) the other. But one can also think of more elaborate ones, where for instance a sampling method can be used to optimize the choice of the incident wave at each iteration step.The latter point is closely related to the design of so called “focusing incident waves” (which are for instance the basis of applications of the time-reversal principle). In the frequency regime, these incident waves can be constructed from the eigenvalue decomposition of the data operator used by sampling methods. The theoretical and numerical investigations of these aspects are still not completely understood for electromagnetic or elastodynamic problems.

Other topological optimization methods, like the homogenization method or the topological gradient method, can also be used, each one provides particular advantages in specific configurations. It is evident that the development of these methods is very suited to inverse problems and provide substantial advantage compared to classical shape optimization methods based on boundary variation. Their applications to inverse problems has not been fully investigated. The efficiency of these optimization methods can also be increased for adequate asymptotic configurations. For instance small amplitude homogenization method can be used as an efficient relaxation method for the inverse problem in the presence of small contrasts. On the other hand, the topological gradient method has shown to perform well in localizing small inclusions with only one iteration.

A broader perspective would be the extension of the above mentioned techniques to time-dependent cases. Taking into account data in time domain is important for many practical applications, such as imaging in cluttered media, the design of absorbing coatings or also crash worthiness in the case of structural design.

For the identification problem, one would like to also have information on the physical properties of the targets. Of course optimization methods is a tool of choice for these problems. However, in some applications only a qualitative information is needed and obtaining it in a cheaper way can be performed using asymptotic theories combined with sampling methods. We also refer here to the use of so called transmission eigenvalues as qualitative indicators for non destructive testing of dielectrics.

We are also interested in parameter identification problems arising in diffusion-type problems. Our research here is mostly motivated by applications to the imaging of biological tissues with the technique of Diffusion Magnetic Resonance Imaging (DMRI). Roughly speaking DMRI gives a measure of the average distance travelled by water molecules in a certain medium and can give useful information on cellular structure and structural change when the medium is biological tissue. In particular, we would like to infer from DMRI measurements changes in the cellular volume fraction occurring upon various physiological or pathological conditions as well as the average cell size in the case of tumor imaging. The main challenges here are 1) correctly model measured signals using diffusive-type time-dependent PDEs 2) numerically handle the complexity of the tissues 3) use the first two to identify physically relevant parameters from measurements. For the last point we are particularly interested in constructing reduced models of the multiple-compartment Bloch-Torrey partial differential equation using homogenization methods.

ECUADOR Project-Team

3. Research Program

3.1. Algorithmic Differentiation

Participants: Laurent Hascoët, Valérie Pascual, Ala Taftaf.

algorithmic differentiation (AD, aka Automatic Differentiation) Transformation of a program, that returns a new program that computes derivatives of the initial program, i.e. some combination of the partial derivatives of the program's outputs with respect to its inputs.

adjoint Mathematical manipulation of the Partial Derivative Equations that define a problem, obtaining new differential equations that define the gradient of the original problem's solution.

Algorithmic Differentiation (AD) differentiates *programs*. The input of AD is a source program P that, given some $X \in \mathbb{R}^n$, returns some $Y = F(X) \in \mathbb{R}^m$, for a differentiable F. AD generates a new source program P' that, given X, computes some derivatives of F [14].

The resulting P' reuses the control of P. For any given control, P is equivalent to a sequence of instructions, which is identified with a composition of vector functions. Thus, if

$$\begin{array}{rcl} P & \text{is} & \{I_1; I_2; \cdots I_p;\}, \\ F & \text{then is} & f_p \circ f_{p-1} \circ \cdots \circ f_1, \end{array} \tag{1}$$

where each f_k is the elementary function implemented by instruction I_k. AD applies the chain rule to obtain derivatives of F. Calling X_k the values of all variables after instruction I_k, i.e. $X_0 = X$ and $X_k = f_k(X_{k-1})$, the Jacobian of F is

$$F'(X) = f'_p(X_{p-1}) \,.\, f'_{p-1}(X_{p-2}) \,.\, \cdots \,.\, f'_1(X_0) \tag{2}$$

which can be mechanically written as a sequence of instructions I'_k. Combining the I'_k with the control of P yields P', and therefore this differentiation is piecewise.

AD can be generalized to higher level derivatives, Taylor series, etc. In practice, many applications only need cheaper projections of $F'(X)$ such as:

- **Sensitivities**, defined for a given direction $\dot{X}$ in the input space as:

$$F'(X).\dot{X} = f'_p(X_{p-1}) \,.\, f'_{p-1}(X_{p-2}) \,.\, \cdots \,.\, f'_1(X_0) \,.\, \dot{X} \quad . \tag{3}$$

  This expression is easily computed from right to left, interleaved with the original program instructions. This is the *tangent mode* of AD.

- **Adjoints**, defined after transposition (F'^*), for a given weighting $\overline{Y}$ of the outputs as:

$$F'^*(X).\overline{Y} = f'^*_1(X_0).f'^*_2(X_1). \cdots .f'^*_{p-1}(X_{p-2}).f'^*_p(X_{p-1}).\overline{Y} \quad . \tag{4}$$

  This expression is most efficiently computed from right to left, because matrix×vector products are cheaper than matrix×matrix products. This defines the *adjoint mode* of AD, most effective for optimization, data assimilation [28], adjoint problems [23], or inverse problems.

Adjoint-mode AD turns out to make a very efficient program, at least theoretically [25]. The computation time required for the gradient is only a small multiple of the run-time of P. It is independent from the number of parameters n. In contrast, computing the same gradient with the *tangent mode* would require running the tangent differentiated program n times.

However, the X_k are required in the *inverse* of their computation order. If the original program *overwrites* a part of X_k, the differentiated program must restore X_k before it is used by $f'^*_{k+1}(X_k)$. Therefore, the central research problem of adjoint-mode AD is to make the X_k available in reverse order at the cheapest cost, using strategies that combine storage, repeated forward computation from available previous values, or even inverted computation from available later values.

Another research issue is to make the AD model cope with the constant evolution of modern language constructs. From the old days of Fortran77, novelties include pointers and dynamic allocation, modularity, structured data types, objects, vectorial notation and parallel communication. We keep developing our models and tools to handle these new constructs.

3.2. Static Analysis and Transformation of programs

Participants: Laurent Hascoët, Valérie Pascual, Ala Taftaf.

abstract syntax tree Tree representation of a computer program, that keeps only the semantically significant information and abstracts away syntactic sugar such as indentation, parentheses, or separators.

control flow graph Representation of a procedure body as a directed graph, whose nodes, known as basic blocks, each contain a sequence of instructions and whose arrows represent all possible control jumps that can occur at run-time.

abstract interpretation Model that describes program static analysis as a special sort of execution, in which all branches of control switches are taken concurrently, and where computed values are replaced by abstract values from a given *semantic domain*. Each particular analysis gives birth to a specific semantic domain.

data flow analysis Program analysis that studies how a given property of variables evolves with execution of the program. Data Flow analysis is static, therefore studying all possible run-time behaviors and making conservative approximations. A typical data-flow analysis is to detect, at any location in the source program, whether a variable is initialized or not.

data dependence analysis Program analysis that studies the itinerary of values during program execution, from the place where a value is defined to the places where it is used, and finally to the place where it is overwritten. The collection of all these itineraries is stored as *Def-Use and Use-Def chains* or as a *data dependence graph*, and data flow analysis most often rely on this graph.

data dependence graph Directed graph that relates accesses to program variables, from the write access that defines a new value to the read accesses that use this value, and from the read accesses to the write access that overwrites this value. Dependences express a partial order between operations, that must be preserved to preserve the program's result.

The most obvious example of a program transformation tool is certainly a compiler. Other examples are program translators, that go from one language or formalism to another, or optimizers, that transform a program to make it run better. AD is just one such transformation. These tools use sophisticated analysis [15]. These tools share their technological basis. More importantly, there are common mathematical models to specify and analyze them.

An important principle is *abstraction*: the core of a compiler should not bother about syntactic details of the compiled program. The optimization and code generation phases must be independent from the particular input programming language. This is generally achieved using language-specific *front-ends* and *back-ends*. Abstraction can go further: the internal representation becomes more language independent, and semantic constructs can be unified. Analysis can then concentrate on the semantics of a small set of constructs. We advocate an internal representation composed of three levels.

- At the top level is the *call graph*, whose nodes are modules and procedures. Arrows relate nodes that call or import one another. Recursion leads to cycles.
- At the middle level is the *flow graph*, one per procedure. It captures the control flow between atomic instructions. Loops lead to cycles.
- At the lowest level are abstract *syntax trees* for the individual atomic instructions. Semantic transformations can benefit from the representation of expressions as directed acyclic graphs, sharing common sub-expressions.

To each level belong symbol tables, nested to capture scoping.

Static program analysis can be defined on this internal representation, which is largely language independent. The simplest analyses on trees can be specified with inference rules [18], [26], [16]. But many analyses are more complex, and better defined on graphs than on trees. This is the case for *data-flow analyses*, that look for run-time properties of variables. Since flow graphs may be cyclic, these global analyses generally require an iterative resolution. *Data flow equations* is a practical formalism to describe data-flow analyses. Another formalism is described in [19], which is more precise because it can distinguish separate *instances* of instructions. However it is still based on trees, and its cost forbids application to large codes. *Abstract Interpretation* [20] is a theoretical framework to study complexity and termination of these analyses.

Data flow analyses must be carefully designed to avoid or control combinatorial explosion. At the call graph level, they can run bottom-up or top-down, and they yield more accurate results when they take into account the different call sites of each procedure, which is called *context sensitivity*. At the flow graph level, they can run forwards or backwards, and yield more accurate results when they take into account only the possible execution flows resulting from possible control, which is called *flow sensitivity*.

Even then, data flow analyses are limited, because they are static and thus have very little knowledge of actual run-time values. Far before reaching the very theoretical limit of *undecidability*, one reaches practical limitations to how much information one can infer from programs that use arrays [32], [21] or pointers. In general, conservative *over-approximations* are always made that lead to derivative code that is less efficient than possibly achievable.

3.3. Algorithmic Differentiation and Scientific Computing

Participants: Alain Dervieux, Laurent Hascoët, Bruno Koobus.

linearization In Scientific Computing, the mathematical model often consists of Partial Derivative Equations, that are discretized and then solved by a computer program. Linearization of these equations, or alternatively linearization of the computer program, predict the behavior of the model when small perturbations are applied. This is useful when the perturbations are effectively small, as in acoustics, or when one wants the sensitivity of the system with respect to one parameter, as in optimization.

adjoint state Consider a system of Partial Derivative Equations that define some characteristics of a system with respect to some input parameters. Consider one particular scalar characteristic. Its sensitivity, (or gradient) with respect to the input parameters can be defined as the solution of "adjoint" equations, deduced from the original equations through linearization and transposition. The solution of the adjoint equations is known as the adjoint state.

Scientific Computing provides reliable simulations of complex systems. For example it is possible to simulate the steady or unsteady 3D air flow around a plane that captures the physical phenomena of shocks and turbulence. Next comes optimization, one degree higher in complexity because it repeatedly simulates and applies optimization steps until an optimum is reached. We focus on gradient-based optimization.

We investigate several approaches to obtain the gradient, between two extremes:

- One can write an *adjoint system* of mathematical equations, then discretize it and program it by hand. This is mathematically sound [23], but very costly in development time. It also does not produce an exact gradient of the discrete function, and this can be a problem if using optimization methods based on descent directions.
- One can apply adjoint-mode AD (*cf*3.1) on the program that discretizes and solves the direct system. This gives in fact the adjoint of the discrete function computed by the program. Theoretical results [22] guarantee convergence of these derivatives when the direct program converges. This approach is highly mechanizable, but leads to massive use of storage and may require code transformation by hand [27], [30] to reduce memory usage.

If for instance the model is steady, or more generally when the computation uses a Fixed-Point iteration, tradeoffs exist between these two extremes [24], [17] that combine low storage consumption with possible automated adjoint generation. We advocate incorporating them into the AD model and into the AD tools.

GAMMA3 Project-Team (section vide)

IPSO Project-Team

3. Research Program

3.1. Structure-preserving numerical schemes for solving ordinary differential equations

Participants: François Castella, Philippe Chartier, Erwan Faou, Vilmart Gilles.

ordinary differential equation, numerical integrator, invariant, Hamiltonian system, reversible system, Lie-group system

In many physical situations, the time-evolution of certain quantities may be written as a Cauchy problem for a differential equation of the form

$$\begin{aligned} y'(t) &= f(y(t)), \\ y(0) &= y_0. \end{aligned} \tag{5}$$

For a given y_0, the solution $y(t)$ at time t is denoted $\varphi_t(y_0)$. For fixed t, φ_t becomes a function of y_0 called the *flow* of (1). From this point of view, a numerical scheme with step size h for solving (1) may be regarded as an approximation Φ_h of φ_h. One of the main questions of *geometric integration* is whether *intrinsic* properties of φ_t may be passed on to Φ_h.

This question can be more specifically addressed in the following situations:

3.1.1. Reversible ODEs

The system (1) is said to be ρ-reversible if there exists an involutive linear map ρ such that

$$\rho \circ \varphi_t = \varphi_t^{-1} \circ \rho = \varphi_{-t} \circ \rho. \tag{6}$$

It is then natural to require that Φ_h satisfies the same relation. If this is so, Φ_h is said to be *symmetric*. Symmetric methods for reversible systems of ODEs are just as much important as *symplectic* methods for Hamiltonian systems and offer an interesting alternative to symplectic methods.

3.1.2. ODEs with an invariant manifold

The system (1) is said to have an invariant manifold g whenever

$$\mathcal{M} = \{y \in \mathbb{R}^n; g(y) = 0\} \tag{7}$$

is kept *globally* invariant by φ_t. In terms of derivatives and for sufficiently differentiable functions f and g, this means that

$$\forall\, y \in \mathcal{M},\, g'(y)f(y) = 0.$$

As an example, we mention Lie-group equations, for which the manifold has an additional group structure. This could possibly be exploited for the space-discretisation. Numerical methods amenable to this sort of problems have been reviewed in a recent paper [60] and divided into two classes, according to whether they use g explicitly or through a projection step. In both cases, the numerical solution is forced to live on the manifold at the expense of some Newton's iterations.

3.1.3. Hamiltonian systems

Hamiltonian problems are ordinary differential equations of the form:

$$\begin{array}{rcl} \dot{p}(t) & = & -\nabla_q H(p(t), q(t)) \quad \in \quad \mathbb{R}^d \\ \dot{q}(t) & = & \nabla_p H(p(t), q(t)) \quad \in \quad \mathbb{R}^d \end{array} \tag{8}$$

with some prescribed initial values $(p(0), q(0)) = (p_0, q_0)$ and for some scalar function H, called the Hamiltonian. In this situation, H is an invariant of the problem. The evolution equation (4) can thus be regarded as a differential equation on the manifold

$$\mathcal{M} = \{(p, q) \in \mathbb{R}^d \times \mathbb{R}^d; H(p, q) = H(p_0, q_0)\}.$$

Besides the Hamiltonian function, there might exist other invariants for such systems: when there exist d invariants in involution, the system (4) is said to be *integrable*. Consider now the parallelogram P originating from the point $(p, q) \in \mathbb{R}^{2d}$ and spanned by the two vectors $\xi \in \mathbb{R}^{2d}$ and $\eta \in \mathbb{R}^{2d}$, and let $\omega(\xi, \eta)$ be the sum of the *oriented* areas of the projections over the planes (p_i, q_i) of P,

$$\omega(\xi, \eta) = \xi^T J \eta,$$

where J is the *canonical symplectic* matrix

$$J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix}.$$

A continuously differentiable map g from $\mathbb{R}^{2d}$ to itself is called symplectic if it preserves ω, i.e. if

$$\omega(g'(p, q)\xi, g'(p, q)\eta) = \omega(\xi, \eta).$$

A fundamental property of Hamiltonian systems is that their exact flow is symplectic. Integrable Hamiltonian systems behave in a very remarkable way: as a matter of fact, their invariants persist under small perturbations, as shown in the celebrated theory of Kolmogorov, Arnold and Moser. This behavior motivates the introduction of *symplectic* numerical flows that share most of the properties of the exact flow. For practical simulations of Hamiltonian systems, symplectic methods possess an important advantage: the error-growth as a function of time is indeed linear, whereas it would typically be quadratic for non-symplectic methods.

3.1.4. Differential-algebraic equations

Whenever the number of differential equations is insufficient to determine the solution of the system, it may become necessary to solve the differential part and the constraint part altogether. Systems of this sort are called differential-algebraic systems. They can be classified according to their index, yet for the purpose of this expository section, it is enough to present the so-called index-2 systems

$$\begin{array}{rcl} \dot{y}(t) & = & f(y(t), z(t)), \\ 0 & = & g(y(t)), \end{array} \tag{9}$$

where initial values $(y(0), z(0)) = (y_0, z_0)$ are given and assumed to be consistent with the constraint manifold. By constraint manifold, we imply the intersection of the manifold

$$\mathcal{M}_1 = \{y \in \mathbb{R}^n, g(y) = 0\}$$

and of the so-called hidden manifold

$$\mathcal{M}_2 = \{(y,z) \in \mathbb{R}^n \times \mathbb{R}^m, \frac{\partial g}{\partial y}(y) f(y,z) = 0\}.$$

This manifold $\mathcal{M} = \mathcal{M}_1 \bigcap \mathcal{M}_2$ is the manifold on which the exact solution $(y(t), z(t))$ of (5) lives.

There exists a whole set of schemes which provide a numerical approximation lying on $\mathcal{M}_1$. Furthermore, this solution can be projected on the manifold $\mathcal{M}$ by standard projection techniques. However, it it worth mentioning that a projection destroys the symmetry of the underlying scheme, so that the construction of a symmetric numerical scheme preserving $\mathcal{M}$ requires a more sophisticated approach.

3.2. Highly-oscillatory systems

Participants: François Castella, Philippe Chartier, Nicolas Crouseilles, Erwan Faou, Florian Méhats, Mohammed Lemou, Gilles Vilmart.

second-order ODEs, oscillatory solutions, Schrödinger and wave equations, step size restrictions.

In applications to molecular dynamics or quantum dynamics for instance, the right-hand side of (1) involves *fast* forces (short-range interactions) and *slow* forces (long-range interactions). Since *fast* forces are much cheaper to evaluate than *slow* forces, it seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

A typical model of highly-oscillatory systems is the second-order differential equations

$$\ddot{q} = -\nabla V(q) \tag{10}$$

where the potential $V(q)$ is a sum of potentials $V = W + U$ acting on different time-scales, with $\nabla^2 W$ positive definite and $\|\nabla^2 W\| >> \|\nabla^2 U\|$. In order to get a bounded error propagation in the linearized equations for an explicit numerical method, the step size must be restricted according to

$$h\omega < C,$$

where C is a constant depending on the numerical method and where ω is the highest frequency of the problem, i.e. in this situation the square root of the largest eigenvalue of $\nabla^2 W$. In applications to molecular dynamics for instance, *fast* forces deriving from W (short-range interactions) are much cheaper to evaluate than *slow* forces deriving from U (long-range interactions). In this case, it thus seems highly desirable to design numerical methods for which the number of evaluations of slow forces is not (at least not too much) affected by the presence of fast forces.

Another prominent example of highly-oscillatory systems is encountered in quantum dynamics where the Schrödinger equation is the model to be used. Assuming that the Laplacian has been discretized in space, one indeed gets the *time*-dependent Schrödinger equation:

$$i\dot{\psi}(t) = \frac{1}{\varepsilon} H(t)\psi(t), \tag{11}$$

where $H(t)$ is finite-dimensional matrix and where ε typically is the square-root of a mass-ratio (say electron/ion for instance) and is small ($\varepsilon \approx 10^{-2}$ or smaller). Through the coupling with classical mechanics ($H(t)$ is obtained by solving some equations from classical mechanics), we are faced once again with two different time-scales, 1 and ε. In this situation also, it is thus desirable to devise a numerical method able to advance the solution by a time-step $h > \varepsilon$.

3.3. Geometric schemes for the Schrödinger equation

Participants: François Castella, Philippe Chartier, Erwan Faou, Florian Méhats, Gilles Vilmart.

Schrödinger equation, variational splitting, energy conservation.

Given the Hamiltonian structure of the Schrödinger equation, we are led to consider the question of energy preservation for time-discretization schemes.

At a higher level, the Schrödinger equation is a partial differential equation which may exhibit Hamiltonian structures. This is the case of the time-dependent Schrödinger equation, which we may write as

$$i\varepsilon \frac{\partial \psi}{\partial t} = H\psi, \tag{12}$$

where $\psi = \psi(x,t)$ is the wave function depending on the spatial variables $x = (x_1, \cdots, x_N)$ with $x_k \in \mathbb{R}^d$ (e.g., with $d = 1$ or 3 in the partition) and the time $t \in \mathbb{R}$. Here, ε is a (small) positive number representing the scaled Planck constant and i is the complex imaginary unit. The Hamiltonian operator H is written

$$H = T + V$$

with the kinetic and potential energy operators

$$T = -\sum_{k=1}^{N} \frac{\varepsilon^2}{2m_k} \Delta_{x_k} \quad \text{and} \quad V = V(x),$$

where $m_k > 0$ is a particle mass and Δ_{x_k} the Laplacian in the variable $x_k \in \mathbb{R}^d$, and where the real-valued potential V acts as a multiplication operator on ψ.

The multiplication by i in (8) plays the role of the multiplication by J in classical mechanics, and the energy $\langle \psi | H | \psi \rangle$ is conserved along the solution of (8), using the physicists' notations $\langle u | A | u \rangle = \langle u, Au \rangle$ where $\langle \ , \ \rangle$ denotes the Hermitian L^2-product over the phase space. In quantum mechanics, the number N of particles is very large making the direct approximation of (8) very difficult.

The numerical approximation of (8) can be obtained using projections onto submanifolds of the phase space, leading to various PDEs or ODEs: see [64], [63] for reviews. However the long-time behavior of these approximated solutions is well understood only in this latter case, where the dynamics turns out to be finite dimensional. In the general case, it is very difficult to prove the preservation of qualitative properties of (8) such as energy conservation or growth in time of Sobolev norms. The reason for this is that backward error analysis is not directly applicable for PDEs. Overwhelming these difficulties is thus a very interesting challenge.

A particularly interesting case of study is given by symmetric splitting methods, such as the Strang splitting:

$$\psi_1 = \exp\left(-i(\delta t)V/2\right) \exp\left(i(\delta t)\Delta\right) \exp\left(-i(\delta t)V/2\right)\psi_0 \tag{13}$$

where δt is the time increment (we have set all the parameters to 1 in the equation). As the Laplace operator is unbounded, we cannot apply the standard methods used in ODEs to derive long-time properties of these schemes. However, its projection onto finite dimensional submanifolds (such as Gaussian wave packets space or FEM finite dimensional space of functions in x) may exhibit Hamiltonian or Poisson structure, whose long-time properties turn out to be more tractable.

3.4. High-frequency limit of the Helmholtz equation

Participant: François Castella.

waves, Helmholtz equation, high oscillations.

The Helmholtz equation models the propagation of waves in a medium with variable refraction index. It is a simplified version of the Maxwell system for electro-magnetic waves.

The high-frequency regime is characterized by the fact that the typical wavelength of the signals under consideration is much smaller than the typical distance of observation of those signals. Hence, in the high-frequency regime, the Helmholtz equation at once involves highly oscillatory phenomena that are to be described in some asymptotic way. Quantitatively, the Helmholtz equation reads

$$i\alpha_\varepsilon u_\varepsilon(x) + \varepsilon^2 \Delta_x u_\varepsilon + n^2(x) u_\varepsilon = f_\varepsilon(x). \tag{14}$$

Here, ε is the small adimensional parameter that measures the typical wavelength of the signal, $n(x)$ is the space-dependent refraction index, and $f_\varepsilon(x)$ is a given (possibly dependent on ε) source term. The unknown is $u_\varepsilon(x)$. One may think of an antenna emitting waves in the whole space (this is the $f_\varepsilon(x)$), thus creating at any point x the signal $u_\varepsilon(x)$ along the propagation. The small $\alpha_\varepsilon > 0$ term takes into account damping of the waves as they propagate.

One important scientific objective typically is to describe the high-frequency regime in terms of *rays* propagating in the medium, that are possibly refracted at interfaces, or bounce on boundaries, etc. Ultimately, one would like to replace the true numerical resolution of the Helmholtz equation by that of a simpler, asymptotic model, formulated in terms of rays.

In some sense, and in comparison with, say, the wave equation, the specificity of the Helmholtz equation is the following. While the wave equation typically describes the evolution of waves between some initial time and some given observation time, the Helmholtz equation takes into account at once the propagation of waves over *infinitely long* time intervals. Qualitatively, in order to have a good understanding of the signal observed in some bounded region of space, one readily needs to be able to describe the propagative phenomena in the whole space, up to infinity. In other words, the "rays" we refer to above need to be understood from the initial time up to infinity. This is a central difficulty in the analysis of the high-frequency behaviour of the Helmholtz equation.

3.5. From the Schrödinger equation to Boltzmann-like equations

Participant: François Castella.

Schrödinger equation, asymptotic model, Boltzmann equation.

The Schrödinger equation is the appropriate way to describe transport phenomena at the scale of electrons. However, for real devices, it is important to derive models valid at a larger scale.

In semi-conductors, the Schrödinger equation is the ultimate model that allows to obtain quantitative information about electronic transport in crystals. It reads, in convenient adimensional units,

$$i\partial_t \psi(t,x) = -\frac{1}{2}\Delta_x \psi + V(x)\psi, \tag{15}$$

where $V(x)$ is the potential and $\psi(t,x)$ is the time- and space-dependent wave function. However, the size of real devices makes it important to derive simplified models that are valid at a larger scale. Typically, one wishes to have kinetic transport equations. As is well-known, this requirement needs one to be able to describe "collisions" between electrons in these devices, a concept that makes sense at the macroscopic level, while it does not at the microscopic (electronic) level. Quantitatively, the question is the following: can one obtain the Boltzmann equation (an equation that describes collisional phenomena) as an asymptotic model for the Schrödinger equation, along the physically relevant micro-macro asymptotics? From the point of view of modelling, one wishes here to understand what are the "good objects", or, in more technical words, what are the relevant "cross-sections", that describe the elementary collisional phenomena. Quantitatively, the Boltzmann equation reads, in a simplified, linearized, form :

$$\partial_t f(t,x,v) = \int_{\mathbf{R}^3} \sigma(v,v')\ [f(t,x,v') - f(t,x,v)]dv'. \tag{16}$$

Here, the unknown is $f(x,v,t)$, the probability that a particle sits at position x, with a velocity v, at time t. Also, $\sigma(v,v')$ is called the cross-section, and it describes the probability that a particle "jumps" from velocity v to velocity v' (or the converse) after a collision process.

MATHERIALS Team

3. Research Program

3.1. Research Program

Quantum Chemistry aims at understanding the properties of matter through the modeling of its behavior at a subatomic scale, where matter is described as an assembly of nuclei and electrons. At this scale, the equation that rules the interactions between these constitutive elements is the Schrödinger equation. It can be considered (except in few special cases notably those involving relativistic phenomena or nuclear reactions) as a universal model for at least three reasons. First it contains all the physical information of the system under consideration so that any of the properties of this system can in theory be deduced from the Schrödinger equation associated to it. Second, the Schrödinger equation does not involve any empirical parameters, except some fundamental constants of Physics (the Planck constant, the mass and charge of the electron, ...); it can thus be written for any kind of molecular system provided its chemical composition, in terms of natures of nuclei and number of electrons, is known. Third, this model enjoys remarkable predictive capabilities, as confirmed by comparisons with a large amount of experimental data of various types. On the other hand, using this high quality model requires working with space and time scales which are both very tiny: the typical size of the electronic cloud of an isolated atom is the Angström (10^{-10} meters), and the size of the nucleus embedded in it is 10^{-15} meters; the typical vibration period of a molecular bond is the femtosecond (10^{-15} seconds), and the characteristic relaxation time for an electron is 10^{-18} seconds. Consequently, Quantum Chemistry calculations concern very short time (say 10^{-12} seconds) behaviors of very small size (say 10^{-27} m^3) systems. The underlying question is therefore whether information on phenomena at these scales is useful in understanding or, better, predicting macroscopic properties of matter. It is certainly not true that *all* macroscopic properties can be simply upscaled from the consideration of the short time behavior of a tiny sample of matter. Many of them derive from ensemble or bulk effects, that are far from being easy to understand and to model. Striking examples are found in solid state materials or biological systems. Cleavage, the ability of minerals to naturally split along crystal surfaces (e.g. mica yields to thin flakes), is an ensemble effect. Protein folding is also an ensemble effect that originates from the presence of the surrounding medium; it is responsible for peculiar properties (e.g. unexpected acidity of some reactive site enhanced by special interactions) upon which vital processes are based. However, it is undoubtedly true that *many* macroscopic phenomena originate from elementary processes which take place at the atomic scale. Let us mention for instance the fact that the elastic constants of a perfect crystal or the color of a chemical compound (which is related to the wavelengths absorbed or emitted during optic transitions between electronic levels) can be evaluated by atomic scale calculations. In the same fashion, the lubricative properties of graphite are essentially due to a phenomenon which can be entirely modeled at the atomic scale. It is therefore reasonable to simulate the behavior of matter at the atomic scale in order to understand what is going on at the macroscopic one. The journey is however a long one. Starting from the basic principles of Quantum Mechanics to model the matter at the subatomic scale, one finally uses statistical mechanics to reach the macroscopic scale. It is often necessary to rely on intermediate steps to deal with phenomena which take place on various *mesoscales*. It may then be possible to couple one description of the system with some others within the so-called *multiscale* models. The sequel indicates how this journey can be completed focusing on the first smallest scales (the subatomic one), rather than on the larger ones. It has already been mentioned that at the subatomic scale, the behavior of nuclei and electrons is governed by the Schrödinger equation, either in its time dependent form or in its time independent form. Let us only mention at this point that

- both equations involve the quantum Hamiltonian of the molecular system under consideration; from a mathematical viewpoint, it is a self-adjoint operator on some Hilbert space; *both* the Hilbert space and the Hamiltonian operator depend on the nature of the system;
- also present into these equations is the wavefunction of the system; it completely describes its state; its L^2 norm is set to one.

The time dependent equation is a first order linear evolution equation, whereas the time-independent equation is a linear eigenvalue equation. For the reader more familiar with numerical analysis than with quantum mechanics, the linear nature of the problems stated above may look auspicious. What makes the numerical simulation of these equations extremely difficult is essentially the huge size of the Hilbert space: indeed, this space is roughly some symmetry-constrained subspace of $L^2(\mathbb{R}^d)$, with $d = 3(M + N)$, M and N respectively denoting the number of nuclei and the number of electrons the system is made of. The parameter d is already 39 for a single water molecule and rapidly reaches 10^6 for polymers or biological molecules. In addition, a consequence of the universality of the model is that one has to deal at the same time with several energy scales. In molecular systems, the basic elementary interaction between nuclei and electrons (the two-body Coulomb interaction) appears in various complex physical and chemical phenomena whose characteristic energies cover several orders of magnitude: the binding energy of core electrons in heavy atoms is 10^4 times as large as a typical covalent bond energy, which is itself around 20 times as large as the energy of a hydrogen bond. High precision or at least controlled error cancellations are thus required to reach chemical accuracy when starting from the Schrödinger equation. Clever approximations of the Schrödinger problems are therefore needed. The main two approximation strategies, namely the Born-Oppenheimer-Hartree-Fock and the Born-Oppenheimer-Kohn-Sham strategies, end up with large systems of coupled *nonlinear* partial differential equations, each of these equations being posed on $L^2(\mathbb{R}^3)$. The size of the underlying functional space is thus reduced at the cost of a dramatic increase of the mathematical complexity of the problem: nonlinearity. The mathematical and numerical analysis of the resulting models has been the major concern of the team for a long time. In the recent years, while part of the activity still follows this path, the focus has progressively shifted to problems at other scales. Such problems are described in the following sections.

MC2 Team

3. Research Program

3.1. Introduction

We are mainly concerned with complex fluid mechanics problems. The complexity consists of the rheological nature of the fluids (non newtonian fluids), of the coupling phenomena (in shape optimization problems), of the geometry (micro-channels) or of multi-scale phenomena arising in turbulence or in tumor growth modeling. Our goal is to understand these phenomena and to simulate and/or to control them. The subject is wide and we will restrict ourselves to three directions: the first one consists in studying low Reynolds number interface problems in multi-fluid flows with applications to complex fluids, microfluidics and biology - the second one deals with numerical simulation of Newtonian fluid flows with emphasis on the coupling of methods to obtain fast solvers.

Even if we deal with several kinds of applications, there is a strong scientific core at each level of our project. Concerning the model, we are mainly concerned with incompressible flows and we work with the classical description of incompressible fluid dynamics. For the numerical methods, we use the penalization method to describe the obstacles or the boundary conditions for high Reynolds flows, for shape optimization, for interface problems in biology or in microfluidics. This allows us to use only cartesian meshes. Moreover, we use the level-set method for interface problems, for shape optimization and for fluid structure interaction. Finally, for the implementation, strong interaction exists between the members of the team and the modules of the numerical codes are used by all the team and we want to build the platform **eLYSe** to systematize this approach.

3.2. Multi-fluid flows and application for complex fluids, microfluidics

Participants: Angelo Iollo, Charles-Henri Bruneau, Thierry Colin, Mathieu Colin, Kévin Santugini.

Multi-fluid flows,microfluidics

By a complex fluid, we mean a fluid containing some mesoscopic objects, i.e. structures whose size is intermediate between the microscopic size and the macroscopic size of the experiment. The aim is to study complex fluids containing surfactants in large quantities. It modifies the viscosity properties of the fluids and surface-tension phenomena can become predominant.

Microfluidics is the study of fluids in very small quantities, in micro-channels (a micro-channel is typically 1 cm long with a section of 50 μ m$\times$ 50 μ m). They are many advantages of using such channels. First, one needs only a small quantity of liquid to analyze the phenomena. Furthermore, very stable flows and quite unusual regimes may be observed, which enables to perfom more accurate measurements. The idea is to couple numerical simulations with experiments to understand the phenomena, to predict the flows and compute some quantities like viscosity coefficients for example. Flows in micro-channels are often at low Reynolds numbers. The hydrodynamical part is therefore stable. However, the main problem is to produce real 3D simulations covering a large range of situations. For example we want to describe diphasic flows with surface tension and sometimes surface viscosity. Surface tension enforces the stability of the flow. The size of the channel implies that one can observe some very stable phenomena. For example, using a "T" junction, a very stable interface between two fluids can be observed. In a cross junction, one can also have formation of droplets that travel along the channel. Some numerical difficulties arise from the surface tension term. With an explicit discretization of this term, a restrictive stability condition appears for very slow flows [77]. Our partner is the LOF, a Rhodia-Bordeaux 1-CNRS laboratory.

One of the main points is the wetting phenomena at the boundary. Note that the boundary conditions are fundamental for the description of the flow since the channels are very shallow. The wetting properties cannot be neglected at all. Indeed, for the case of a two non-miscible fluids system, if one considers no-slip boundary conditions, then since the interface is driven by the velocity of the fluids, it shall not move on the boundary. The experiments shows that this is not true: the interface is moving and in fact all the dynamics start from the boundary and then propagate in the whole volume of fluids. Even with low Reynolds numbers, the wetting effects can induce instabilities and are responsible of hardly predictable flows. Moreover, the fluids that are used are often visco-elastic and exhibit "unusual" slip length. Therefore, we cannot use standard numerical codes and have to adapt the usual numerical methods to our case to take into account the specificities of our situations. In Johana Pinilla's thesis the Cox law has been implemented successfully to allow the interface to move properly between two Newtonian fluids of various viscosity or one Newtonian and one non-Newtonian fluid. Moreover, we want to obtain reliable models and simulations that can be as simple as possible and that can be used by our collaborators. As a summary, the main specific points of the physics are: the multi-fluid simulations at low Reynolds number, the wetting problems and the surface tension that are crucial, the 3D characteristic of the flows, the boundary conditions that are fundamental due to the size of the channels. We need to handle complex fluids. Our collaborators in this lab are H. Bordiguel, J.-B. Salmon, P. Guillot, A. Colin.

The evolution of non-newtonian flows in webs of micro-channels are therefore useful to understand the mixing of oil, water and polymer for enhanced oil recovery for example. Complex fluids arising in cosmetics are also of interest. We also need to handle mixing processes.

3.3. Cancer modeling

Participants: Sébastien Benzekry, Thierry Colin, Angelo Iollo, Clair Poignard, Olivier Saut, Lisl Weynans.

Tumor growth, cancer, metastasis

As in microfluidics, the growth of a tumor is a low Reynolds number flow. Several kinds of interfaces are present (membranes, several populations of cells,...) The biological nature of the tissues impose the use of different models in order to describe the evolution of tumor growth. The complexity of the geometry, of the rheological properties and the coupling with multi-scale phenomena is high but not far away from those encountered in microfluidics and the models and methods are close.

The challenge is twofold. On one hand, we wish to understand the complexity of the coupling effects between the different levels (cellular, genetic, organs, membranes, molecular). Trying to be exhaustive is of course hopeless, however it is possible numerically to isolate some parts of the evolution in order to better understand the interactions. Another strategy is to test *in silico* some therapeutic innovations. An example of such a test is given in [88] where the efficacy of radiotherapy is studied and in [89] where the effects of anti-invasive agents is investigated. It is therefore useful to model a tumor growth at several stage of evolution. The macroscopic continuous model is based on Darcy's law which seems to be a good approximation to describe the flow of the tumor cells in the extra-cellular matrix [54], [78], [79]. It is therefore possible to develop a two-dimensional model for the evolution of the cell densities. We formulate mathematically the evolution of the cell densities in the tissue as advection equations for a set of unknowns representing the density of cells with position (x, y) at time t in a given cycle phase. Assuming that all cells move with the same velocity given by Darcy's law and applying the principle of mass balance, one obtains the advection equations with a source term given by a cellular automaton. We assume diffusion for the oxygen and the diffusion constant depends on the density of the cells. The source of oxygen corresponds to the spatial location of blood vessels. The available quantities of oxygen interact with the proliferation rate given by the cellular automaton [88].

Another axis of these theoretical investigations is the study of several processes in cancer biology (with a major focus on metastasis) for applications in theoretical and experimental onco-biology as well as preclinical and clinical studies. This axis regroups several projects for which our approach can be decomposed into three steps. First, we base ourselves on a detailed study of the particular biological process, based on the available literature and in close collaboration with biologists and the available data. In a second step, we reduce the biological dynamics to its more essential components and build mathematical models able to simulate the process, to address the particular biological question under investigation and to give nontrivial insights on the overall complex combination of these dynamics. Eventually, the last step consists in confronting the models to the data, using statistical parameter estimation methods, in order to identify theories or hypothesis that could or could not have generated the data and thus improve the biological understanding or identify optimal therapeutic strategies.

A forthcoming investigation in cancer treatment simulation is the influence of the electrochemotherapy [83] on the tumor growth. Electrochemotherapy consists in imposing to the malignant tumor high voltage electric pulses so that the plasma membrane of carcinoma cells is permeabilized. Biologically active molecules such as bleomycin, which usually cannot diffuse through the membrane, may then be internalized. A work in progress (C.Poignard [87] in collaboration with the CNRS lab of physical vectorology at the Institut Gustave Roussy) consists in modelling electromagnetic phenomena at the cell scale. A coupling between the microscopic description of the electroporation of cells and its influence on the global tumor growth at the macroscopic scale is expected. Another key point is the parametrization of the models in order to produce image-based simulations.

The second challenge is more ambitious. Mathematical models of cancer have been extensively developed with the aim of understanding and predicting tumor growth and the effects of treatments. In vivo modeling of tumors is limited by the amount of information available. However, in the last few years there have been dramatic increases in the range and quality of information available from non-invasive imaging methods, so that several potentially valuable imaging measurements are now available to quantitatively measure tumor growth, assess tumor status as well as anatomical or functional details. Using different methods such as the CT scan, magnetic resonance imaging (MRI), or positron emission tomography (PET), it is now possible to evaluate and define tumor status at different levels: physiological, molecular and cellular.

In this context, the present project aims at supporting the decision process of oncologists in the definition of therapeutic protocols via quantitative methods. The idea is to build mathematically and physically sound phenomenological models that can lead to patient-specific full-scale simulations, starting from data collected typically through medical imagery like CT scans, MRIs and PET scans or by quantitative molecular biology for leukemia. Our ambition is to provide medical doctors with patient-specific tumor growth models able to estimate, on the basis of previously collected data and within the limits of phenomenological models, the evolution at subsequent times of the pathology and possibly the response to the therapies.

The final goal is to provide numerical tools in order to help to answer to the crucial questions for a clinician:
When to start a treatment?
When to change a treatment?
When to stop a treatment?
Also we intend to incorporate real-time model information for improving the precision and effectiveness of non-invasive or micro-invasive tumor ablation techniques like acoustic hyperthermia, electroporation, radiofrequency or cryo-ablation.

We will specifically focus on the following pathologies: Lung and liver metastasis of a distant tumor
Low grade and high grade gliomas, meningiomas
Chronic myelogenous leukemia
These pathologies have been chosen because of the existing collaborations between the applied mathematics department of University of Bordeaux and the Institut Bergonié.

Our approach. Our approach is deterministic and spatial: it is based on solving an inverse problem based on imaging data. Models are of partial differential equation (PDE) type. They are coupled with a process of data assimilation based on imaging. We already have undertaken test cases on patients that are followed at Bergonié for lung metastases of thyroid tumors. These patients have a slowly evolving, asymptomatic metastatic disease, monitored by CT scans. On two thoracic images relative to successive times, the volume of the tumor under investigation is extracted by segmentation. To test our method, we chose patients without treatment and for whom we had at least three successive.

3.4. Newtonian fluid flows simulations and their analysis

Participants: Charles-Henri Bruneau, Angelo Iollo, Iraj Mortazavi, Michel Bergmann, Lisl Weynans.

Simulation, Analysis

It is very exciting to model complex phenomena for high Reynolds flows and to develop methods to compute the corresponding approximate solutions, however a well-understanding of the phenomena is necessary. Classical graphic tools give us the possibility to visualize some aspects of the solution at a given time and to even see in some way their evolution. Nevertheless in many situations it is not sufficient to understand the mechanisms that create such a behavior or to find the real properties of the flow. It is then necessary to carefully analyze the flow, for instance the vortex dynamics or to identify the coherent structures to better understand their impact on the whole flow behavior.
The various numerical methods used or developed to approximate the flows depend on the studied phenomenon. Our goal is to compute the most reliable method for each situation.
The first method, which is affordable in 2D, consists in a directly solving of the genuine Navier-Stokes equations in primitive variables (velocity-pressure) on Cartesian domains [64]. The bodies, around which the flow has to be computed are modeled using the penalization method (also named Brinkman-Navier-Stokes equations). This is an immersed boundary method in which the bodies are considered as porous media with a very small intrinsic permeability [55]. This method is very easy to handle as it consists only in adding a mass term U/K in the momentum equations. The boundary conditions imposed on artificial boundaries of the computational domains avoid any reflections when vortices cross the boundary. To make the approximation efficient enough in terms of CPU time, a multi-grid solver with a cell by cell Gauss-Seidel smoother is used.
The second type of methods is the vortex method. It is a Lagrangian technique that has been proposed as an alternative to more conventional grid-based methods. Its main feature is that the inertial nonlinear term in the flow equations is implicitly accounted for by the transport of particles. The method thus avoids to a large extent the classical stability/accuracy dilemma of finite-difference or finite-volume methods. This has been demonstrated in the context of computations for high Reynolds number laminar flows and for turbulent flows at moderate Reynolds numbers [72]. This method has recently enabled us to obtain new results concerning the three-dimensional dynamics of cylinder wakes.
The third method is to develop reduced order models (ROM) based on a Proper Orthogonal Decomposition (POD) [80]. The POD consists in approximating a given flow field $U(x,t)$ with the decomposition

$$U(x,t) = \sum_i a_i(t)\phi_i(x),$$

where the basis functions are empirical in the sense that they derive from an existing data base given for instance by one of the methods above. Then the approximation of Navier-Stokes equations for instance is reduced to solving a low-order dynamical system that is very cheap in terms of CPU time. Nevertheless the ROM can only restitute what is contained in the basis. Our challenge is to extend its application in order to make it an actual prediction tool.
The fourth method is a finite volume method on cartesian grids to simulate compressible Euler or Navier Stokes Flows in complex domains. An immersed boundary-like technique is developed to take into account boundary conditions around the obstacles with order two accuracy.

3.5. Flow control and shape optimization

Participants: Charles-Henri Bruneau, Angelo Iollo, Iraj Mortazavi, Michel Bergmann.

Flow Control, Shape Optimization

Flow simulations, optimal design and flow control have been developed these last years in order to solve real industrial problems : vortex trapping cavities with CIRA (Centro Italiano Ricerche Aerospaziali), reduction of vortex induced vibrations on deep sea riser pipes with IFP (Institut Français du Pétrole), drag reduction of a ground vehicle with Renault or in-flight icing with Bombardier and Pratt-Wittney are some examples of possible applications of these researches. Presently the recent creation of the competitiveness cluster on aeronautics, space and embedded systems (AESE) based also in Aquitaine provides the ideal environment to extend our applied researches to the local industrial context. There are two main streams: the first need is to produce direct numerical simulations, the second one is to establish reliable optimization procedures.
In the next subsections we will detail the tools we will base our work on, they can be divided into three points: to find the appropriate devices or actions to control the flow; to determine an effective system identification technique based on the trace of the solution on the boundary; to apply shape optimization and system identification tools to the solution of inverse problems found in object imaging and turbomachinery.

3.5.1. Control of flows

There are mainly two approaches: passive (using passive devices on some specific parts that modify the shear forces) or active (adding locally some energy to change the flow) control.

The passive control consists mainly in adding geometrical devices to modify the flow. One idea is to put a porous material between some parts of an obstacle and the flow in order to modify the shear forces in the boundary layer. This approach may pose remarkable difficulties in terms of numerical simulation since it would be necessary, a priori, to solve two models: one for the fluid, one for the porous medium. However, by using the penalization method it becomes a feasible task [60]. This approach has been now used in several contexts and in particular in the frame of a collaboration with IFP to reduce vortex induced vibrations [61]. Another technique we are interested in is to inject minimal amounts of polymers into hydrodynamic flows in order to stabilize the mechanisms which enhance hydrodynamic drag.

The active approach is addressed to conceive, implement and test automatic flow control and optimization aiming mainly at two applications : the control of unsteadiness and the control and optimization of coupled systems. Implementation of such ideas relies on several tools. The common challenges are infinite dimensional systems, Dirichlet boundary control, nonlinear tracking control, nonlinear partial state observation.

The bottom-line to obtain industrially relevant control devices is the energy budget. The energy required by the actuators should be less than the energy savings resulting from the control application. In this sense our research team has gained a certain experience in testing several control strategies with a doctoral thesis (E. Creusé) devoted to increasing the lift on a dihedral plane. Indeed the extension of these techniques to real world problems may reveal itself very delicate and special care will be devoted to implement numerical methods which permit on-line computing of actual practical applications. For instance the method can be successful to reduce the drag forces around a ground vehicle and a coupling with passive control is under consideration to improve the efficiency of each control strategy.

3.5.2. System identification

We remark that the problem of deriving an accurate estimation of the velocity field in an unsteady complex flow, starting from a limited number of measurements, is of great importance in many engineering applications. For instance, in the design of a feedback control, a knowledge of the velocity field is a fundamental element in deciding the appropriate actuator reaction to different flow conditions. In other applications it may be necessary or advisable to monitor the flow conditions in regions of space which are difficult to access or where probes cannot be fitted without causing interference problems.

The idea is to exploit ideas similar to those at the basis of the Kalman filter. The starting point is again a Galerkin representation of the velocity field in terms of empirical eigenfunctions. For a given flow, the POD modes can be computed once and for all based on Direct Numerical Simulation (DNS) or on highly resolved experimental velocity fields, such as those obtained by particle image velocimetry. An instantaneous velocity field can thus be reconstructed by estimating the coefficients $a_i(t)$ of its Galerkin representation. One simple approach to estimate the POD coefficients is to approximate the flow measurements in a least square sense, as in [76].

A similar procedure is also used in the estimation based on gappy POD, see [92] and [96]. However, these approaches encounter difficulties in giving accurate estimations when three-dimensional flows with complicated unsteady patterns are considered, or when a very limited number of sensors is available. Under these conditions, for instance, the least squares approach cited above (LSQ) rapidly becomes ill-conditioned. This simply reflects the fact that more and more different flow configurations correspond to the same set of measurements.

Our challenge is to propose an approach that combines a linear estimation of the coefficients $a_i(t)$ with an appropriate non-linear low-dimensional flow model, that can be readily implemented for real time applications.

3.5.3. Shape optimization and system identification tools applied to inverse problems found in object imaging and turbomachinery

We will consider two different objectives. The first is strictly linked to the level set methods that are developed for microfluidics. The main idea is to combine different technologies that are developed with our team: penalization methods, level sets, an optimization method that regardless of the model equation will be able to solve inverse or optimization problems in 2D or 3D. For this we have started a project that is detailed in the research program. See also [67] for a preliminary application.

As for shape optimization in aeronautics, the aeroacoustic optimization problem of propeller blades is addressed by means of an inverse problem and its adjoint equations. This problem is divided into three subtasks:

i) formulation of an inverse problem for the design of propeller blades and determination of the design parameters ii) derivation of an aeroacoustic model able to predict noise levels once the blade geometry and the flow field are given iii) development of an optimization procedure in order to minimize the noise emission by controlling the design parameters.

The main challenge in this field is to move from simplified models [81] to actual 3D model. The spirit is to complete the design performed with a simplified tool with a fully three dimensional inverse problem where the load distribution as well as the geometry of the leading edge are those provided by the meridional plane analysis [91]. A 3D code will be based on the compressible Euler equations and an immersed boundary technique over a cartesian mesh. The code will be implicit and parallel, in the same spirit as what was done for the meridional plane. Further development include the extension of the 3D immersed boundary approach to time-dependent phenomena. This step will allow the designer to take into account noise sources that are typical of internal flows. The task will consist in including time dependent forcing on the inlet and/or outlet boundary under the form of Fourier modes and in computing the linearized response of the system. The optimization will then be based on a direct approach, i.e., an approach where the control is the geometry of the boundary. The computation of the gradient is performed by an adjoint method, which will be a simple "byproduct" of the implicit solver. The load distribution as well as the leading edge geometry obtained by the meridional plane approach will be considered as constraints of the optimization, by projection of the gradient on the constraint tangent plane. These challenges will be undertaken in collaboration with Politecnico di Torino and EC Lyon.

MEPHYSTO Team

3. Research Program

3.1. From statistical physics to continuum mechanics

Whereas numerical methods in nonlinear elasticity are well-developed and reliable, constitutive laws used for rubber in practice are phenomenological and generally not very precise. On the contrary, at the scale of the polymer-chain network, the physics of rubber is very precisely described by statistical physics. The main challenge in this field is to understand how to derive macroscopic constitutive laws for rubber-like materials from statistical physics.

At the continuum level, rubber is modelled by an energy E defined as the integral over a domain D of $\mathbb{R}^d$ of some energy density W depending only locally on the gradient of the deformation u: $E(u) = \int_D W(\nabla u(x))dx$. At the microscopic level (say 100nm), rubber is a network of cross-linked and entangled polymer chains (each chain is made of a sequence of monomers). At this scale the physics of polymer chains is well-understood in terms of statistical mechanics: monomers thermally fluctuate according to the Boltzmann distribution [46]. The associated Hamiltonian of a network is typically given by a contribution of the polymer chains (using self-avoiding random bridges) and a contribution due to steric effects (rubber is packed and monomers are surrounded by an excluded volume). The main challenge is to understand how this statistical physics picture yields rubber elasticity. Treloar assumed in [56] that for a piece of rubber undergoing some macroscopic deformation, the cross-links do not fluctuate and follow the macroscopic deformation, whereas between two cross-links, the chains fluctuate. This is the so-called affine assumption. Treloar's model is in rather good agreement with mechanical experiments in small deformation. In large deformation however, it overestimates the stress. A natural possibility to relax Treloar's model consists in relaxing the affine assumption while keeping the network description, which allows one to distinguish between different rubbers. This can be done by assuming that the deformation of the cross-links minimizes the free energy of the polymer chains, the deformation being fixed at the boundary of the macroscopic domain D. This gives rise to a "variational model". The analysis of the asymptotic behavior of this model as the typical length of a polymer chain vanishes has the same flavor as the homogenization theory of integral functionals in nonlinear elasticity (see [41], [52] in the periodic setting, and [42] in the random setting).

Our aim is to relate qualitatively and quantitatively the (precise but unpractical) statistical physics picture to explicit macroscopic constitutive laws that can be used for practical purposes.

In collaboration with R. Alicandro (Univ. Cassino, Italy) and M. Cicalese (Univ. Munich, Germany), A. Gloria analyzed in [1] the (asymptotic) Γ-convergence of the variational model for rubber, in the case when the polymer chain network is represented by some ergodic random graph. The easiest such graph is the Delaunay tessellation of a point set generated as follows: random hard spheres of some given radius ρ are picked randomly until the domain is jammed (the so-called random parking measure of intensity ρ). With M. Penrose (Univ. Bath, UK), A. Gloria studied this random graph in this framework [6]. With P. Le Tallec (Mechanics department, Ecole polytechnique, France), M. Vidrascu (project-team REO, Inria Paris-Rocquencourt), and A. Gloria introduced and tested in [15] a numerical algorithm to approximate the homogenized energy density, and observed that this model compares well to rubber elasticity qualitatively.

These preliminary results show that the variational model has the potential to explain qualitatively and quantitatively how rubber elasticity emerges from polymer physics. In order to go further and obtain more quantitative results and rigorously justify the model, we have to address several questions of analysis, modelling, scientific computing, inverse problems, and physics.

3.2. Quantitative stochastic homogenization

Whereas the approximation of homogenized coefficients is an easy task in periodic homogenization, this is a highly nontrivial task for stochastic coefficients. This is in order to analyze numerical approximation methods of the homogenized coefficients that F. Otto (MPI for mathematics in the sciences, Leipzig, Germany) and A. Gloria obtained the first quantitative results in stochastic homogenization [4]. The development of a complete stochastic homogenization theory seems to be ripe for the analysis and constitutes the second major objective of this section.

In order to develop a quantitative theory of stochastic homogenization, one needs to quantitatively understand the corrector equation (3). Provided A is stationary and ergodic, it is known that there exists a unique random field ϕ_ξ which is a distributional solution of (3) almost surely, such that $\nabla\phi_\xi$ is a stationary random field with bounded second moment $\langle|\nabla\phi_\xi|^2\rangle < \infty$, and with $\phi(0) = 0$. Soft arguments do not allow to prove that ϕ_ξ may be chosen stationary (this is wrong in dimension $d = 1$). In [4], [5] F. Otto and A. Gloria proved that, in the case of discrete elliptic equations with iid conductances, there exists a unique stationary corrector ϕ_ξ with vanishing expectation in dimension $d > 2$. Although it cannot be bounded, it has bounded finite moments of any order:

$$\langle|\phi_\xi|^q\rangle < \infty \text{ for all } q \geq 1. \tag{17}$$

They also proved that the variance of spatial averages of the energy density $(\xi + \nabla\phi_\xi) \cdot A(\xi + \nabla\phi_\xi)$ on balls of radius R decays at the rate R^{-d} of the central limit theorem. These are the *first optimal quantitative results* in stochastic homogenization.

The proof of these results, which is inspired by [53], is based on the insight that coefficients such as the Poisson random inclusions are special in the sense that the associated probability measure satisfies a spectral gap estimate. Combined with elliptic regularity theory, this spectral gap estimate quantifies ergodicity in stochastic homogenization. This systematic use of tools from statistical physics has opened the way to the quantitative study of stochastic homogenization problems, which we plan to fully develop.

3.3. Nonlinear Schrödinger equations

As well known, the (non)linear Schrödinger equation

$$\partial_t\varphi(t,x) = -\Delta\varphi(t,x) + \lambda V(x)\varphi(t,x) + g|\varphi|^2\varphi(t,x), \quad \varphi(0,x) = \varphi_0(x) \tag{18}$$

with coupling constants $g \in \mathbb{R}, \lambda \in \mathbb{R}_+$ and real potential V (possibly depending also on time) models many phenomena of physics.

When in the equation (5) above one sets $\lambda = 0, g \neq 0$, one obtains the nonlinear (focusing of defocusing) Schrödinger equation. It is used to model light propagation in optical fibers. In fact, it then takes the following form:

$$i\partial_z\varphi(t,z) = -\beta(z)\partial_t^2\varphi(t,z) + \gamma(z)|\varphi(t,z)|^2\varphi(z,t), \tag{19}$$

where β and γ are functions that characterize the physical properties of the fiber, t is time and z the position along the fiber. Several issues are of importance here. Two that will be investigated within the MEPHYSTO project are: the influence of a periodic modulation of the fiber parameters β and γ and the generation of so-called “rogue waves” (which are solutions of unusually high amplitude) in such systems.

If $g = 0, \lambda \neq 0$, V is a random potential, and φ_0 is deterministic, this is the standard random Schrödinger equation describing for example the motion of an electron in a random medium. The main issue in this setting is the determination of the regime of Anderson localization, a property characterized by the boundedness in time of the second moment $\int x^2 |\varphi(t,x)|^2 dx$ of the solution. If this second moment remains bounded in time, the solution is said to be localized. Whereas it is known that the solution is localized in one dimension for all (suitable) initial data, both localized and delocalized solutions exist in dimension 3 and it remains a major open problem today to prove this, cf. [44].

If now $g \neq 0, \lambda \neq 0$ and V is still random, but $|g| \ll \lambda$, a natural question is whether, and in which regime, one-dimensional Anderson localization perdures. Indeed, Anderson localization can be affected by the presence of the nonlinearity, which corresponds to an interaction between the electrons or atoms. Much numerical and some analytical work has been done on this issue (see for example [47] for a recent work at PhLAM, Laser physics department, Univ. Lille 1), but many questions remain, notably on the dependence of the result on the initial conditions, which, in a nonlinear system, may be very complex. The cold atoms team of PhLAM (Garreau-Szriftgiser) is currently setting up an experiment to analyze the effect of the interactions in a Bose-Einstein condensate on a closely related localization phenomenon called "dynamical localization", in the kicked rotor, see below.

3.4. Dynamical localization and kicked rotors

The kicked rotor is a unitary discrete time dynamics proposed in the seventies in the context of studies on quantum chaos, and used recently as a "quantum simulator" for the Anderson model. It is a quantum equivalent of the standard map and is obtained by integrating a time-dependent linear Schrödinger equation with a time-periodic, very singular (delta comb) potential. It continues to pose considerable mathematical challenges, in particular the so-called "quantum suppression of classical chaos" in the presence of a strong potential, which remains an open problem from the mathematical point of view. It can be rephrased as follows: show that the H^1 norm of the solution is uniformly bounded in time (see [36] for more background). In more recent years, the question has arisen how the behavior of this system would change in the presence of a nonlinear term in the Schrödinger equation.

This problem displays both numerical and analytical challenges, in particular because of the difficulty to obtain long time simulations of the system and because of the presence of instabilities due to the nonlinearity. Preliminary theoretical results motivate some conjectures on the behavior of these systems, that we plan to validate empirically in a first step. Indeed, reliable long-time simulations of the system should allow us to get more insight into the behavior of the exact solutions in the unstable cases. One of the main difficulties for the numerical simulation is the intrinsic instability of the system, which magnifies quite rapidly the numerical error due to machine precision. This requires the use of multiprecision techniques in order to handle reasonably long times, even for moderate nonlinearities, and of the transparent boundary conditions recently introduced by members of the former SIMPAF project-team.

MOKAPLAN Team

3. Research Program

3.1. Context

Optimal Mass Transportation is a mathematical research topic which started two centuries ago with Monge's work on "des remblais et déblais". This engineering problem consists in minimizing the transport cost between two given mass densities. In the 40's, Kantorovich [64] solved the dual problem and interpreted it as an economic equilibrium. The *Monge-Kantorovich* problem became a specialized research topic in optimization and Kantorovich obtained the 1975 Nobel prize in economics for his contributions to resource allocations problems. Following the seminal discoveries of Brenier in the 90's [35], Optimal Transportation has received renewed attention from mathematical analysts and the Fields Medal awarded in 2010 to C. Villani, who gave important contributions to Optimal Transportation and wrote the modern reference monograph [84], arrived at a culminating moment for this theory. Optimal Mass Transportation is today a mature area of mathematical analysis with a constantly growing range of applications (see below).

In the modern Optimal Mass Transportation problem, we are given two probability measures or "mass" densities : $d\rho_i(x_i)(=\rho_i(x_i)\,dx_i),\ i=0,1$ such that $\rho_i\ge 0,\ \int_{X_0}\rho_0(x_0)dx_0=\int_{X_1}\rho_1(x_1)dx_1=1$, $X_i\subset R^n$. They are often referred to, respectively, source and target densities, support or spaces. The problem is the minimization of a *transportation cost*, $\mathcal{I}(M)=\int_{X_0}c(x,M(x))\,\rho_0(x)dx$ where c is a displacement *ground cost*, over all *volume preserving maps*$M\in\mathcal{MM}=\{M:X_0\to X_1,\ M_\#d\rho_0=d\rho_1\}$. Assuming that M is a diffeomorphism, this is equivalent to the *Jacobian equation*$det(DM(x))\rho_1(M(x))=\rho_0(x)$. Most of the modern Optimal Mass Transportation theory has been developed for the Euclidean distance squared cost $c(x,y)=\|x-y)\|^2$ while the historic monge cost was the simple distance $c(x,y)=\|x-y\|$.

In the Euclidean distance squared ground cost, the problem is well posed and in the seminal work of Brenier [36], the optimal map is characterized as the gradient of a convex potential ϕ^* : $\mathcal{I}(\nabla\phi^*(x))=\min_{M\in\mathcal{M}}\mathcal{I}(M)$. A formal substitution in the Jacobian equation gives the Monge-Ampère equation $det(D^2\phi^*)\rho_1(\nabla\phi^*(x))=\rho_0(x)$ complemented by the *second boundary value* condition $\nabla\phi^*(X_0)\subset X_1$. Caffarelli [41] used this result to extend the regularity theory for the Monge-Ampère equation. He noticed in particular that Optimal Mass Transportation solutions, now called *Brenier solutions*, may have discontinuous gradients when the target density support X_1 is non convex and are therefore weaker than the Monge-Ampère potentials associated to Alexandrov measures (see [60] for a review of the different notions of Monge-Ampère solutions). The value function $\sqrt{\mathcal{I}(\nabla\phi^*)}$ is also known to be the *Wasserstein distance*$W_2(\rho_0,\rho_1)$ on the space of probability densities, see [84]. The *Computational Fluid Dynamic* formulation proposed by Brenier and Benamou in [2] introduces a time extension of the domain and leads to a convex but non smooth optimization problem : $\mathcal{I}(\nabla\phi^*)=\min_{(\rho,V)\in\mathcal{C}}\displaystyle\int_0^1\int_X\frac{1}{2}\rho(t,x)\,\|V(t,x)\|^2\,dx\,dt$. with constraints : $\mathcal{C}=\{(\rho,V),\ \text{s.t}\ \partial_t\rho+div(\rho V)=0,\ \rho(\{0,1\},.)=\rho_{\{0,1\}}(.)\}$. The time curves $t\to\rho(t,.)$ are geodesics between ρ_0 and ρ_1 for the Wasserstein distance. This formulation is a limit case of *Mean Fields games* [65], a large class of economic models introduced by Lasry and Lions. The Wasserstein distance and its connection to Optimal Mass Transportation also appears in the construction of semi-discrete Gradient Flows. This notion known as *JKO gradient flows* after its authors in [62] is a popular tool to study non-linear diffusion equations : the implicit Euler scheme $\rho^{dt}_{k+1}=argmin_{\rho(.)}\,F(\rho(.))+\frac{1}{2\,dt}W_2(\rho(.),\rho^{dt}_k)^2$ can be shown to converge $\rho^{dt}_k(.))\to\rho^*(t,.)$ as $dt\to 0$ to the solution of the non linear continuity equation $\partial_t\rho^*+div(\rho^*\,\nabla(-\frac{\partial F}{\partial\rho}(\rho^*)))=0,\ \rho^*(0,.)=\rho^{dt}_0(.)$. The prototypical example is given by $F(\rho)=\int_X\rho(x)\,\log(\rho(x))+\rho(x)\,V(x)\,dx$ which corresponds to the classical Fokker-Planck equation. Extensions of the ground cost c have been actively studied recently, some are mentioned in the application section. Technical results culminating with the *Ma-Trudinger-Wang* condition [68] which gives necessary condition on c for the regularity of the solution of the Optimal Mass Transportation problem. More recently attention has risen on multi marginal Optimal Mass Transportation [59] and has been systematically studied

in [76] [79] [77] [78]. The data consists in an arbitrary (and even infinite) number N of densities (the marginals) and the ground cost is defined on a product space $c(x_0, x_1, ..., x_{n-1})$ of the same dimension. Several interesting applications belong to this class of models (see below).
Our focus is on numerical methods in Optimal Mass Transportation and applications. The simplest way to build a numerical method is to consider sum of dirac masses $\rho_0 = \sum_{i=1}^N \delta_{A_i} \quad \rho_1 = \sum_{j=1}^N \delta_{B_j}$. In that case the Optimal Mass Transportation problem reduces to combinatorial optimisation *assigment problem* between the points $\{A_i\}$s and $\{B_i\}$s : $\min_{\sigma \in Permut(1,N)} \frac{1}{N} \sum_{i=1}^N C_{i,\sigma(i)} C_{i,j} = \|A_i - B_j\|^2$. The complexity of the best (Hungarian or Auction) algorithm, see [33] for example, is $O(N^{\frac{5}{2}})$. An interesting variant is obtained when only the target measure is discrete. For instance $X_0 = \{\|x\| < 1\},\ \rho_0 = \frac{1}{|X_0|} \quad \rho_1 = \frac{1}{N} \sum_{j=1}^N \delta_{y_j}$. It corresponds to the notion of Pogorelov solutions of the Monge-Ampère equation [80] and is also linked to Minkowski problem [31]. The optimal map is piecewise constant and the slopes are known. More precisely there exists N polygonal cells C_j such that $X_0 = \cup_j C_j$, $|C_j| = \frac{1}{N}$ and $\nabla \phi^*|_{C_j} = y_j$. Pogorelov proposed a constructive algorithm to build these solutions which has been refined and extended in particular in [50] [74] [72] [71]. The complexity is still not linear : $O(N^2 logN)$.
For general densities data, the original optimization problem is not tractable because of the volume preserving constraint on the map. Kantorovich dual formulation is a linear program but with a large number of constraints set over the product of the source and target space $X_0 \times X_1$. The CFD formulation [2]. preserves the convexity of the objective function and transforms the volume preserving constraint into a linear continuity equation (using a change of variable). We obtained a convex but non smooth optimization problem solved using an Augmented Lagrangian method [53], as originally proposed in [2]. It has been reinterpreted recently in the framework of proximal algorithms [75]. This approach is robust and versatile and has been reimplemented many times. It remains a first order optimization method and converges slowly. The cost is also increased by the additional artificial time dimension. An empirical complexity is $O(N^3 LogN)$ where N is the space discretization of the density. Several variants and extension of these methods have been implemented, in particular in [39] [30]. It is the only provably convergent method to compute Brenier (non C^1) solutions.
When interested in slightly more regular solutions which correspond to the assumption that the target support is convex, the recent *wide stencil* monotone finite difference scheme for the Monge-Ampère equation [55] can be adapted to the Optimal Mass Transportation problem. This is the topic of [7]. This approach is extremely fast as a Newton algorithm can be used to solve the discrete system. Numerical studies confirm this with a linear empirical complexity.

For other costs, JKO schemes, multi marginal extensions, partial transport ... efficient numerical methods are to be invented.

NACHOS Project-Team

3. Research Program

3.1. Scientific foundations

The teams focuses on physical applications dealing with electromagnetic or elastodynamic wave propagation in interaction with heterogeneous media and irregularly shaped structures. The underlying wave propagation phenomena can be purely unsteady or they can be periodic (because the imposed source term follows a time-harmonic evolution). In this context, the research activities undertaken by the team aim at developing innovative numerical methodologies putting the emphasis on several features:

- **Accuracy**. The foreseen numerical methods should rely on discretization techniques that best fit to the geometrical characteristics of the problems at hand. Methods based on unstructured, locally refined, even non-conforming, simplicial meshes are particularly attractive in this regard. In addition, the proposed numerical methods should also be capable to accurately describe the underlying physical phenomena that may involve highly variable space and time scales. Both objectives are generally addressed by studying so-called hp-adaptive solution strategies which combine h-adaptivity using local refinement/coarsening of the mesh and p-adaptivity using adaptive local variation of the interpolation order for approximating the solution variables. However, for physical problems involving strongly heterogeneous or high contrast propagation media, such a solution strategy may not be sufficient. Then, for dealing accurately with these situations, one has to design numerical methods that specifically address the multiscale nature of the underlying physical phenomena.
- **Numerical efficiency**. The simulation of unsteady problems most often relies on explicit time integration schemes. Such schemes are constrained by a stability criterion, linking some space and time discretization parameters, that can be very restrictive when the underlying mesh is highly non-uniform (especially for locally refined meshes). For realistic 3d problems, this can represent a severe limitation with regards to the overall computing time. One possible overcoming solution consists in resorting to an implicit time scheme in regions of the computational domain where the underlying mesh size is very small, while an explicit time scheme is applied elsewhere in the computational domain. The resulting hybrid explicit-implicit time integration strategy raises several challenging questions concerning both the mathematical analysis (stability and accuracy, especially for what concern numerical dispersion), and the computer implementation on modern high performance systems (data structures, parallel computing aspects). A second, often considered approach is to devise a local time strategy in the context of a fully explicit time integration scheme. Beside, when considering time-harmonic wave propagation problems, numerical efficiency is mainly linked to the solution of the system of algebraic equations resulting from the discretization in space of the underlying PDE model. Various strategies exist ranging from the more robust and efficient sparse direct solvers to the more flexible and cheaper (in terms of memory resources) iterative methods. Current trends tend to show that the ideal candidate will be a judicious mix of both approaches by relying on domain decomposition principles.
- **Computational efficiency**. Realistic 3d wave propagation problems involve the processing of very large volumes of data. The latter results from two combined parameters: the size of the mesh i.e the number of mesh elements, and the number of degrees of freedom per mesh element which is itself linked to the degree of interpolation and to the number of physical variables (for systems of partial differential equations). Hence, numerical methods must be adapted to the characteristics of modern parallel computing platforms taking into account their hierarchical nature (e.g multiple processors and multiple core systems with complex cache and memory hierarchies). In addition, appropriate parallelization strategies need to be designed that combine SIMD and MIMD programming paradigms.

From the methodological point of view, the research activities of the team are concerned with four main topics: (1) high order finite element type methods on unstructured or hybrid structured/unstructured meshes for the discretization of the considered systems of PDEs, (2) efficient time integration strategies for dealing with grid induced stiffness when using non-uniform (locally refined) meshes, (3) numerical treatment of complex propagation media models (e.g. physical dispersion models), (4) algorithmic adaptation to modern high performance computing platforms.

3.2. High order discretization methods

3.2.1. The Discontinuous Galerkin method

The Discontinuous Galerkin method (DG) was introduced in 1973 by Reed and Hill to solve the neutron transport equation. From this time to the 90's a review on the DG methods would likely fit into one page. In the meantime, the Finite Volume approach (FV) has been widely adopted by computational fluid dynamics scientists and has now nearly supplanted classical finite difference and finite element methods in solving problems of nonlinear convection and conservation law systems. The success of the FV method is due to its ability to capture discontinuous solutions which may occur when solving nonlinear equations or more simply, when convecting discontinuous initial data in the linear case. Let us first remark that DG methods share with FV methods this property since a first order FV scheme may be viewed as a 0th order DG scheme. However a DG method may also be considered as a Finite Element (FE) one where the continuity constraint at an element interface is released. While keeping almost all the advantages of the FE method (large spectrum of applications, complex geometries, etc.), the DG method has other nice properties which explain the renewed interest it gains in various domains in scientific computing as witnessed by books or special issues of journals dedicated to this method [42]- [43]- [44]- [49]:

- It is naturally adapted to a high order approximation of the unknown field. Moreover, one may increase the degree of the approximation in the whole mesh as easily as for spectral methods but, with a DG method, this can also be done very locally. In most cases, the approximation relies on a polynomial interpolation method but the DG method also offers the flexibility of applying local approximation strategies that best fit to the intrinsic features of the modeled physical phenomena.
- When the space discretization is coupled to an explicit time integration scheme, the DG method leads to a block diagonal mass matrix whatever the form of the local approximation (e.g. the type of polynomial interpolation). This is a striking difference with classical, continuous FE formulations. Moreover, the mass matrix may be diagonal if the basis functions are orthogonal.
- It easily handles complex meshes. The grid may be a classical conforming FE mesh, a non-conforming one or even a hybrid mesh made of various elements (tetrahedra, prisms, hexahedra, etc.). The DG method has been proven to work well with highly locally refined meshes. This property makes the DG method more suitable (and flexible) to the design of some hp-adaptive solution strategy.
- It is also flexible with regards to the choice of the time stepping scheme. One may combine the DG spatial discretization with any global or local explicit time integration scheme, or even implicit, provided the resulting scheme is stable.
- It is naturally adapted to parallel computing. As long as an explicit time integration scheme is used, the DG method is easily parallelized. Moreover, the compact nature of DG discretization schemes is in favor of high computation to communication ratio especially when the interpolation order is increased.

As with standard FE methods, a DG method relies on a variational formulation of the continuous problem at hand. However, due to the discontinuity of the global approximation, this variational formulation has to be defined locally, at the element level. Then, a degree of freedom in the design of a DG method stems from the approximation of the boundary integral term resulting from the application of an integration by parts to the element-wise variational form. In the spirit of FV methods, the approximation of this boundary integral term calls for a numerical flux function which can be based on either a centered scheme or an upwind scheme, or a blending between these two schemes.

3.2.2. High order DG methods for wave propagation models

DG methods are et the heart of the activities of the pteam regarding the development of high order discretization schemes for the PDE systems modeling electromagnetic and elatsodynamic wave propagation:

- **Nodal DG methods for time-domain problems**. For the numerical solution of the time-domain Maxwell equations, we have first proposed a non-dissipative high order DGTD (Discontinuous Galerkin Time Domain) method working on unstructured conforming simplicial meshes [19]-[2]. This DG method combines a central numerical flux function for the approximation of the integral term at the interface of two neighboring elements with a second order leap-frog time integration scheme. Moreover, the local approximation of the electromagnetic field relies on a nodal (Lagrange type) polynomial interpolation method. Recent achievements by the team deal with the extension of these methods towards non-conforming meshes and hp-adaptivity [16]-[17], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [6]. A high order DG method has also been proposed for the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [4]-[15].
- **Hybridizable DG (HDG) method for time-domain and time-harmonic problems**. For the numerical treatment of the time-harmonic Maxwell equations, nodal DG methods can also be consiered [7]-[14]. However, such DG formulations are highly expensive, especially for the discretization of 3d problems, because they lead to a large sparse and undefinite linear system of equations coupling all the degrees of freedom of the unknown physical fields. Different attempts have been made in the recent past to improve this situation and one promising strategy has been recently proposed by Cockburn *et al.*[47] in the form of so-called hybridizable DG formulations. The distinctive feature of these methods is that the only globally coupled degrees of freedom are those of an approximation of the solution defined only on the boundaries of the elements. This work is concerned with the study of such Hybridizable Discontinuous Galerkin (HDG) methods for the solution of the system of Maxwell equations in the time-domain when the time integration relies on an implicit scheme, or in the frequency domain. The team has been a precursor in the development of HDG methods for the frequency-domain Maxwell equations [22]-[23].
- **Multiscale DG methods for time-domain problems**. More recently, in the framework of a collaboration with LNCC in Petropolis (Frédéric Valentin), we have started to investigate a family of methods specifically designed for an accurate and efficient numerical treatment of multiscale wave propagation problems. These methods, referred to as Multiscale Hybrid Mixed (MHM) methods, are currently studied in the team for both time-domain electromagnetic and elastodynamic PDE models. They consist in reformulating the mixed variational form of each system into a global (arbitrarily coarse) problem related to a weak formulation of the boundary condition (carried by a Lagrange multiplier that represents e.g. the normal stress tensor in elastodynamic sytems), and a series of small, element-wise, fully decoupled problems resembling to the initial one and related to some well chosen partition of the solution variables on each element. By construction, that methodology is fully parallelizable and recursivity may be used in each local problem as well, making MHM methods belonging to multi-level highly parallelizable methods. Each local problem may be solved using DG or classical Galerkin FE approximations combined with some appropriate time integration scheme (θ-scheme or leap-frog scheme).

3.3. Efficient time integration strategies

The use of unstructured meshes (based on triangles in two space dimensions and tetrahedra in three space dimensions) is an important feature of the DGTD methods developed in the team which can thus easily deal with complex geometries and heterogeneous propagation media. Moreover, DG discretization methods are naturally adapted to local, conforming as well as non-conforming, refinement of the underlying mesh, Most of the existing DGTD methods rely on explicit time integration schemes and lead to block diagonal mass matrices which is often recognized as one of the main advantages with regards to continuous finite element methods. However, explicit DGTD methods are also constrained by a stability condition that can be very restrictive on highly refined meshes and when the local approximation relies on high order polynomial interpolation. There are basically three strategies that can be considered to cure this computational efficiency problem. The first approach is to use an unconditionally stable implicit time integration scheme to overcome the restrictive constraint on the time step for locally refined meshes. In a second approach, a local time stepping strategy is combined with an explicit time integration scheme. In the third approach, the time step size restriction is overcome by using a hybrid explicit-implicit procedure. In this case, one blends a time implicit and a time explicit schemes where only the solution variables defined on the smallest elements are treated implicitly. The first and third options are considered in the team in the framework of DG [6]-[25]-[24] and HDG [20] discretization methods.

3.4. Numerical treatment of complex material models

Towards the general aim of being able to consider concrete physical situations, we are interested in taking into account in the numerical methodologies that we study, a better description of the propagation of waves in realistic media. In the case of electromagnetics, a typical physical phenomenon that one has to consider is *dispersion*. It is present in almost all media and traduces the way the material reacts to the presence of electromagnetic waves. In the presence of an electric field a medium does not react instantaneously and thus presents an electric polarization of the molecules or electrons that itself influences the electric displacement. In the case of a linear homogeneous isotropic media, there is a linear relation between the applied electric field and the polarization. However, above some range of frequencies (depending on the considered material), the dispersion phenomenon cannot be neglected and the relation between the polarization and the applied electric field becomes complex. This is traduced by a frequency-dependent complex permittivity. Several such models for the characterization of the permittivity exist. Concerning biological media, the Debye model is commonly adopted in the presence of water, biological tissues and polymers, so that it already covers a wide range of applications [21]. If one is interested in modeling the dispersion effects on metals on the nanometer scale and at optical frequencies, which are the conditions that one has to deal with in the context of nanoplasmonics, then the Drude or the Drude-Lorentz models are generally adopted [26]. In the context of seismic wave propagation, we are interested by the intrinsic attenuation of the medium. In realistic configurations, for instance in sedimentary basins where the waves are trapped, we can observe site effects due to local geological and geotechnical conditions which result in a strong increase in amplification and duration of the ground motion at some particular locations. During the wave propagation in such media, a part of the seismic energy is dissipated because of anelastic losses relied to the internal friction of the medium. For these reasons, numerical simulations based on the basic assumption of linear elasticity are no more valid since this assumption result in a severe overestimation of amplitude and duration of the ground motion, even when we are not in presence of a site effect, since intrinsic attenuation is not taken into account.

3.5. High performance numerical computing

Beside basic research activities related to the design of numerical methods and resolution algorithms for the wave propagation models at hand, the team is also committed to demonstrate the benefits of the proposed numerical methodologies in the simulation of challenging three-dimensional problems pertaining to computational electromagnetics and computation geoseismics. For such applications, parallel computing is a mandatory path. Nowadays, modern parallel computers most often take the form of clusters of heterogeneous multiprocessor systems, combining multiple core CPUs with accelerator cards (e.g Graphical Processing Units - GPUs), with complex hierarchical distributed-shared memory systems. Developing numerical algorithms that efficiently exploit such high performance computing architectures raises several challenges, especially in the context of a massive parallelism. In this context, current efforts of the team are towards the exploitation of multiple levels of parallelism (computing systems combining CPUs and GPUs) through the study of hierarchical SPMD (Single Program Multiple Data) strategies for the parallelization of unstructured mesh based solvers.

NANO-D Project-Team (section vide)

OPALE Project-Team

3. Research Program

3.1. Functional and numerical analysis of PDE systems

Our common scientific background is the functional and numerical analysis of PDE systems, in particular with respect to nonlinear hyperbolic equations such as conservation laws of gas-dynamics.

Whereas the structure of weak solutions of the Euler equations has been thoroughly discussed in both the mathematical and fluid mechanics literature, in similar hyperbolic models, focus of new interest, such as those related to traffic, the situation is not so well established, except in one space dimension, and scalar equations. Thus, the study of such equations is one theme of emphasis of our research.

The well-developed domain of numerical methods for PDE systems, in particular finite volumes, constitute the sound background for PDE-constrained optimization.

3.2. Numerical optimization of PDE systems

Partial Differential Equations (PDEs), finite volumes/elements, geometrical optimization, optimum shape design, multi-point/multi-criterion/multi-disciplinary optimization, shape parameterization, gradient-based/evolutionary/hybrid optimizers, hierarchical physical/numerical models, Proper Orthogonal Decomposition (POD)

Optimization problems involving systems governed by PDEs, such as optimum shape design in aerodynamics or electromagnetics, are more and more complex in the industrial setting.

In certain situations, the major difficulty resides in the costly evaluation of a functional by means of a simulation, and the numerical method to be used must exploit at best the problem characteristics (regularity or smoothness, local convexity).

In many other cases, several criteria are to be optimized and some are non differentiable and/or non convex. A large set of parameters, sometimes of different types (boolean, integer, real or functional), are to be taken into account, as well as constraints of various types (physical and geometrical, in particular). Additionally, today's most interesting optimization pre-industrial projects are multi-disciplinary, and this complicates the mathematical, physical and numerical settings. Developing *robust optimizers* is therefore an essential objective to make progress in this area of scientific computing.

In the area of numerical optimization algorithms, the project aims at adapting classical optimization methods (simplex, gradient, quasi-Newton) when applicable to relevant engineering applications, as well as developing and testing less conventional approaches such as Evolutionary Strategies (ES), including Genetic or Particle-Swarm Algorithms, or hybrid schemes, in contexts where robustness is a very severe constraint.

In a different perspective, the heritage from the former project Sinus in Finite-Volumes (or -Elements) for nonlinear hyperbolic problems, leads us to examine cost-efficiency issues of large shape-optimization applications with an emphasis on the PDE approximation; of particular interest to us:

- best approximation and shape-parameterization,
- convergence acceleration (in particular by multi-level methods),
- model reduction (e.g. by *Proper Orthogonal Decomposition*),
- parallel and grid computing; etc.

3.3. Geometrical optimization

Jean-Paul Zolesio and Michel Delfour have developed, in particular in their book [6], a theoretical framework for for geometrical optimization and shape control in Sobolev spaces.

In preparation to the construction of sound numerical techniques, their contribution remains a fundamental building block for the functional analysis of shape optimization formulations.

3.4. Integration platforms

Developing grid, cloud and high-performance computing for complex applications is one of the priorities of the IST chapter in the 7th Framework Program of the European Community. One of the challenges of the 21st century in the computer science area lies in the integration of various expertise in complex application areas such as simulation and optimization in aeronautics, automotive and nuclear simulation. Indeed, the design of the reentry vehicle of a space shuttle calls for aerothermal, aerostructure and aerodynamics disciplines which all interact in hypersonic regime, together with electromagnetics. Further, efficient, reliable, and safe design of aircraft involve thermal flows analysis, consumption optimization, noise reduction for environmental safety, using for example aeroacoustics expertise.

The integration of such various disciplines requires powerful computing infrastructures and particular software coupling techniques. Simultaneously, advances in computer technology militate in favor of the use of massively parallel clusters including hundreds of thousands of processors connected by high-speed gigabits/sec networks. This conjunction makes it possible for an unprecedented cross-fertilization of computational methods and computer science. New approaches including evolutionary algorithms, parameterization, multi-hierarchical decomposition lend themselves seamlessly to parallel implementations in such computing infrastructures. This opportunity is being dealt with by the Opale project-team since its very beginning. A software integration platform has been designed by the Opale project-team for the definition, configuration and deployment of multidisciplinary applications on a distributed heterogeneous infrastructure. Experiments conducted within European projects and industrial cooperations using CAST have led to significant performance results in complex aerodynamics optimization test-cases involving multi-elements airfoils and evolutionary algorithms, i.e. coupling genetic and hierarchical algorithms involving game strategies [77].

The main difficulty still remains however in the deployment and control of complex distributed applications by the end-users. Indeed, the deployment of the computing infrastructures and of the applications in such environments still requires specific expertise by computer science specialists. However, the users, which are experts in their particular application fields, e.g. aerodynamics, are not necessarily experts in distributed and grid computing. Being accustomed to Internet browsers, they want similar interfaces to interact with high-performance computing and problem-solving environments. A first approach to solve this problem is to define component-based infrastructures, e.g. the Corba Component Model, where the applications are considered as connection networks including various application codes. The advantage is here to implement a uniform approach for both the underlying infrastructure and the application modules. However, it still requires specific expertise not directly related to the application domains of each particular user. A second approach is to make use of web services, defined as application and support procedures to standardize access and invocation to remote support and application codes. This is usually considered as an extension of Web services to distributed infrastructures. A new approach, which is currently being explored by the Opale project, is the design of a virtual computing environment able to hide the underlying high-performance-computing infrastructures to the users. The team is exploring the use of distributed workflows to define, monitor and control the execution of high-performance simulations on distributed clusters. The platform includes resilience, i.e., fault-tolerance features allowing for resource demanding and erroneous applications to be dynamically restarted safely, without user intervention.

POEMS Project-Team

3. Research Program

3.1. General description

Our activity relies on the existence of boundary value problems established by physicists to model the propagation of waves in various situations. The basic ingredient is a linear partial differential equation of the hyperbolic type, whose prototype is the wave equation (or the Helmholtz equation if time-periodic solutions are considered). Nowadays, the numerical techniques for solving the basic academic problems are well mastered. However, the resolution of complex wave propagation problems close to real applications still poses (essentially open) problems which constitute a real challenge for applied mathematicians. In particular, several difficulties arise when extending the results and the methods from the scalar wave equation to vectorial problems modeling wave propagation in electromagnetism or elastodynamics.

A large part of research in mathematics, when applied to wave propagation problems, is oriented towards the following goals:

- The conception of new numerical methods, more and more accurate and high performing.
- The development of artificial transparent boundary conditions for handling unbounded propagation domains.
- The treatment of more and more complex problems (non local models, non linear models, coupled systems, periodic media).
- The study of specific phenomena such as guided waves and resonances, which raise mathematical questions of spectral theory.
- The development of approximate models via asymptotic analysis with multiple scales (thin layers, boundary or interfaces, small homogeneities, homogenization, ...).
- The development and the analysis of algorithms for inverse problems (in particular for inverse scattering problems) and imaging techniques, using wave phenomena.

3.2. Wave propagation in non classical media

Extraordinary phenomena regarding the propagation of electromagnetic or acoustic waves appear in materials which have non classical properties: materials with a complex periodic microstructure which behave as a material with negative physical parameters, metals which have a negative dielectric permittivity at optical frequencies, magnetized plasmas which present a strongly anisotropic permittivity tensor with eigenvalues of different signs. These non classical materials raise original questions from theoretical and numerical points of view.

The objective is to study the well-posedness in this unusual context where physical parameters are sign-changing. New functional frameworks must be introduced, due, for instance, to hypersingularities of the electromagnetic field which appear at corners of metamaterials. This has of course numerical counterparts. In particular, classical Perfectly Matched Layers are unstable in these dispersive media, and new approaches must be developed.

Two ANR projects (METAMATH and CHROME) are related to this activity.

3.3. Wave propagation in heterogeneous media

One objective is to develop efficient numerical approaches for the propagation of waves in heterogeneous media.

We aim on one hand to improve homogenized modeling of periodic media, by deriving enriched boundary conditions (or transmission conditions if the periodic structure is embedded in a homogeneous matrix) which take into account the boundary layers phenomena.

On the other hand, we like to develop multi-scale numerical methods when the assumption of periodicity on the spatial distribution of the heterogeneities is either relaxed, or even completely lost. The general idea consists in a coupling between a macroscopic solver, based on a coarse mesh, with some microscopic representation of the field. This latter can be obtained by a numerical microscopic solver or by an analytical asymptotic expansion. This leads to two very different approaches which may be relevant for very different applications.

3.4. Spectral theory and modal approaches for waveguides

The study of waveguides is an old and major topic of the team. Concerning the selfadjoint spectral theory for open waveguides, we turned recently to the very important case of periodic media. One objective is to design periodic structures with localized perturbations to create gaps in the spectrum, containing isolating eigenvalues.

Then, we would like to go further in proving the absence of localized modes in non uniform open waveguides. An original approach has been successfully applied to the scalar problem of a 2D junction. The challenge now is to extend these ideas to other configurations: 3D junctions, bent waveguides, vectorial problems...

Besides, we will continue our activity on modal methods for closed waveguides. In particular, we aim at extending the enriched modal method to take into account curvature and rough boundaries.

Finally, we are developing asymptotic models for networks of thin waveguides which arise in several applications (electric networks, simulation of lung, nanophotonics...).

3.5. Inverse problems

Building on the strong expertise of POEMS in the mathematical modeling of waves, most of our contributions aim at improving inverse scattering methodologies.

We acquired some expertise on the so called Linear Sampling Method, from both the theoretical and the practical points of view. Besides, we are working on topological derivative methods, which exploit small-defect asymptotics of misfit functionals and can thus be viewed as an alternative sampling approach, which can take benefit of our expertise on asymptotic methods.

An originality of our activity is to consider inverse scattering in waveguides (the inverse scattering community generally considers only free-space configurations). This is motivated at the same time by specific issues concerning the ill-posedness of the identification process and by applications to non-destructive techniques, for waveguide configurations (cables, pipes, plates etc...).

Lastly, we continue our work on the so-called exterior approach for solving inverse obstacle problems, which associates quasi-reversibility and level set methods. The objective is now to extend it to evolution problems.

3.6. Integral equations

Our activity in this field aims at developing accurate and fast methods for 3D problems.

On one hand, we developed a systematic approach to the analytical evaluation of singular integrals, which arise in the computation of the matrices of integral equations when two elements of the mesh are either touching each other or geometrically close.

On the other hand, POEMS is developing a Fast Multipole Boundary Element Method (FM-BEM) for elastodynamics, for applications to soil-structure interaction or seismology.

Finally, a posteriori error analysis methodologies and adaptivity for boundary integral equation formulations of acoustic, electromagnetic and elastic wave propagation is investigated in the framework of the ANR project RAFFINE.

3.7. Domain decomposition methods

This is a come back to a topic in which POEMS contributed in the 1990's. It is motivated by our collaborations with the CEA-CESTA and the CEA-LIST, for the solution of large problems in time-harmonic electromagnetism and elastodynamics.

We combine in an original manner classical ideas of Domain Decomposition Methods with the specific formulations that we use for wave problems in unbounded domains, taking benefit of the available analytical representations of the solution (integral representation, modal expansion etc...).

APICS Project-Team

3. Research Program

3.1. Introduction

Within the extensive field of inverse problems, much of the research by Apics deals with reconstructing solutions of classical elliptic PDEs from their boundary behavior. Perhaps the simplest example lies with harmonic identification of a stable linear dynamical system: the transfer-function f can be evaluated at a point $i\omega$ of the imaginary axis from the response to a periodic input at frequency ω. Since f is holomorphic in the right half-plane, it satisfies there the Cauchy-Riemann equation $\overline{\partial} f = 0$, and recovering f amounts to solve a Dirichlet problem which can be done in principle using, *e.g.* the Cauchy formula.

Practice is not nearly as simple, for f is only measured pointwise in the pass-band of the system which makes the problem ill-posed [72]. Moreover, the transfer function is usually sought in specific form, displaying the necessary physical parameters for control and design. For instance if f is rational of degree n, then $\overline{\partial} f = \sum_1^n a_j \delta_{z_j}$ where the z_j are its poles and δ_{z_j} is a Dirac unit mass at z_j. Thus, to find the domain of holomorphy (*i.e.* to locate the z_j) amounts to solve a (degenerate) free-boundary inverse problem, this time on the left half-plane. To address such questions, the team has developed a two-step approach as follows.

Step 1: To determine a complete model, that is, one which is defined at every frequency, in a sufficiently versatile function class (*e.g.* Hardy spaces). This ill-posed issue requires regularization, for instance constraints on the behavior at non-measured frequencies.

Step 2: To compute a reduced order model. This typically consists of rational approximation of the complete model obtained in step 1, or phase-shift thereof to account for delays. We emphasize that deriving a complete model in step 1 is crucial to achieve stability of the reduced model in step 2.

Step 1 relates to extremal problems and analytic operator theory, see Section 3.3.1 . Step 2 involves optimization, and some Schur analysis to parametrize transfer matrices of given Mc-Millan degree when dealing with systems having several inputs and outputs, see Section 3.3.2.2 . It also makes contact with the topology of rational functions, in particular to count critical points and to derive bounds, see Section 3.3.2 . Step 2 raises further issues in approximation theory regarding the rate of convergence and the extent to which singularities of the approximant (*i.e.* its poles) tend to singularities of the approximated function; this is where logarithmic potential theory becomes instrumental, see Section 3.3.3 .

Applying a realization procedure to the result of step 2 yields an identification procedure from incomplete frequency data which was first demonstrated in [78] to tune resonant microwave filters. Harmonic identification of nonlinear systems around a stable equilibrium can also be envisaged by combining the previous steps with exact linearization techniques from [36].

A similar path can be taken to approach design problems in the frequency domain, replacing the measured behavior by some desired behavior. However, describing achievable responses in terms of the design parameters is often cumbersome, and most constructive techniques rely on specific criteria adapted to the physics of the problem. This is especially true of filters, the design of which traditionally appeals to polynomial extremal problems [74], [59]. Apics contributed to this area the use of Zolotarev-like problems for multi-band synthesis, although we presently favor interpolation techniques in which parameters arise in a more transparent manner, see Section 3.2.2 .

The previous example of harmonic identification quickly suggests a generalization of itself. Indeed, on identifying $\mathbb{C}$ with $\mathbb{R}^2$, holomorphic functions become conjugate-gradients of harmonic functions, so that harmonic identification is, after all, a special case of a classical issue: to recover a harmonic function on a domain from partial knowledge of the Dirichlet-Neumann data; when the portion of boundary where data are not available is itself unknown, we meet a free boundary problem. This framework for 2-D non-destructive control was first advocated in [64] and subsequently received considerable attention. It makes clear how to state similar problems in higher dimensions and for more general operators than the Laplacian, provided solutions are essentially determined by the trace of their gradient on part of the boundary which is the case for elliptic equations [0] [25], [83]. Such questions are particular instances of the so-called inverse potential problem, where a measure μ has to be recovered from the knowledge of the gradient of its potential (*i.e.*, the field) on part of a hypersurface (a curve in 2-D) encompassing the support of μ. For Laplace's operator, potentials are logarithmic in 2-D and Newtonian in higher dimensions. For elliptic operators with non constant coefficients, the potential depends on the form of fundamental solutions and is less manageable because it is no longer of convolution type. Nevertheless it is a useful concept bringing perspective on how problems could be raised and solved, using tools from harmonic analysis.

Inverse potential problems are severely indeterminate because infinitely many measures within an open set produce the same field outside this set; this phenomenon is called *balayage* [71]. In the two steps approach previously described , we implicitly removed this indeterminacy by requiring in step 1 that the measure be supported on the boundary (because we seek a function holomorphic throughout the right half space), and by requiring in step 2 that the measure be discrete in the left half-plane. The discreteness assumption also prevails in 3-D inverse source problems, see Section 4.2 . Conditions that ensure uniqueness of the solution to the inverse potential problem are part of the so-called regularizing assumptions which are needed in each case to derive efficient algorithms.

To recap, the gist of our approach is to approximate boundary data by (boundary traces of) fields arising from potentials of measures with specific support. Note that it is different from standard approaches to inverse problems, where descent algorithms are applied to integration schemes of the direct problem; in such methods, it is the equation which gets approximated (in fact: discretized).

Along these lines, Apics advocates the use of steps 1 and 2 above, along with some singularity analysis, to approach issues of nondestructive control in 2-D and 3-D [43] [5], [2]. The team is currently engaged in two kinds of generalizations, to be described further in Section 3.2.1 . The first deals with non-constant conductivities in 2-D, where Cauchy-Riemann equations characterizing holomorphic functions are replaced by conjugate Beltrami equations characterizing pseudo-holomorphic functions; next in line are 3-D situations that we begin to consider, see Sections 6.2 and 4.4 . There, we seek applications to inverse free boundary problems such as plasma confinement in the vessel of a tokamak, or inverse conductivity problems like those arising in impedance tomography. The second generalization lies with inverse source problems for the Laplace equation in 3-D, where holomorphic functions are replaced by harmonic gradients; applications are to EEG/MEG and inverse magnetization problems in paleomagnetism, see Section 4.2 .

The approximation-theoretic tools developed by Apics to handle issues mentioned so far are outlined in Section 3.3 . In Section 3.2 to come, we describe in more detail which problems are considered and which applications are targeted.

3.2. Range of inverse problems

3.2.1. Elliptic partial differential equations (PDE)

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By standard properties of conjugate differentials, reconstructing Dirichlet-Neumann boundary conditions for a function harmonic in a plane domain, when these boundary conditions are known already on a subset E of the boundary, is equivalent to recover a holomorphic function in the domain from its boundary values on E. This is the problem raised on the half-plane in step 1 of Section 3.1 . It makes good sense in holomorphic Hardy spaces where functions are entirely determined by their values on boundary subsets of positive linear

[0] There is a subtle difference here between dimension 2 and higher. Indeed, a function holomorphic on a plane domain is defined by its non-tangential limit on a boundary subset of positive linear measure, but there are non-constant harmonic functions in the 3-D ball, C^1 up to the boundary sphere, yet having vanishing gradient on a subset of positive measure of the sphere. Such a "bad" subset, however, cannot have interior points on the sphere.

measure, which is the framework for Problem (P) that we set up in Section 3.3.1 . Such issues naturally arise in nondestructive testing of 2-D (or 3-D cylindrical) materials from partial electrical measurements on the boundary. For instance, the ratio between the tangential and the normal currents (the so-called Robin coefficient) tells one about corrosion of the material. Thus, solving Problem (P) where ψ is chosen to be the response of some uncorroded piece with identical shape yields non destructive testing of a potentially corroded piece of material, part of which is inaccessible to measurements. This was an initial application of holomorphic extremal problems to non-destructive control [56], [60].

Another application by the team deals with non-constant conductivity over a doubly connected domain, the set E being now the outer boundary. Measuring Dirichlet-Neumann data on E, one wants to recover level lines of the solution to a conductivity equation, which is a so-called free boundary inverse problem. For this, given a closed curve inside the domain, we first quantify how constant the solution on this curve. To this effect, we state and solve an analog of Problem (P), where the constraint bears on the real part of the function on the curve (it should be close to a constant there), in a Hardy space of a conjugate Beltrami equation, of which the considered conductivity equation is the compatibility condition (just like the Laplace equation is the compatibility condition of the Cauchy-Riemann system). Subsequently, a descent algorithm on the curve leads one to improve the initial guess. For example, when the domain is regarded as separating the edge of a tokamak's vessel from the plasma (rotational symmetry makes this a 2-D situation), this method can be used to estimate the shape of a plasma subject to magnetic confinement. It was successfully applied, in collaboration with CEA (French nuclear agency) and the University of Nice (JAD Lab.), to data from *Tore Supra* [63]. The procedure is fast because no numerical integration of the underlying PDE is needed, as an explicit basis of solutions to the conjugate Beltrami equation in terms of Bessel functions was found in this case. Generalizing this approach in a more systematic manner to free boundary problems of Bernoulli type, using descent algorithms based on shape-gradient for such approximation-theoretic criteria, is an interesting prospect, still to be pursued.

The piece of work we just mentioned requires defining and studying Hardy spaces of the conjugate-Beltrami equation, which is an interesting topic by itself. For Sobolev-smooth coefficients of exponent greater than 2, this was done in references [4] and [14]. The case of the critical exponent 2 is treated in [34], which apparently provides the first example of well-posedness for the Dirichlet problem in the non-strictly elliptic case: the conductivity may be unbounded or zero on sets of zero capacity and, accordingly, solutions need not be locally bounded.

The 3-D version of step 1 in Section 3.1 is another subject investigated by Apics: to recover a harmonic function (up to a constant) in a ball or a half-space from partial knowledge of its gradient on the boundary. This prototypical inverse problem (*i.e.* inverse to the Cauchy problem for the Laplace equation) often recurs in electromagnetism. At present, Apics is involved with solving instances of this inverse problem arising in two fields, namely medical imaging *e.g.* for electroencephalography (EEG) or magneto-encephalography (MEG), and paleomagnetism (recovery of rocks magnetization) [2], [38], see Section 6.1 . In this connection, we collaborate with two groups of partners: Athena Inria project-team, CHU La Timone, and BESA company on the one hand, Geosciences Lab. at MIT and Cerege CNRS Lab.on the other hand. The question is considerably more difficult than its 2-D counterpart, due mainly to the lack of multiplicative structure for harmonic gradients. Still, considerable progress has been made over the last years using methods of harmonic analysis and operator theory.

The team is further concerned with 3-D generalizations and applications to non-destructive control of step 2 in Section 3.1 . A typical problem is here to localize inhomogeneities or defaults such as cracks, sources or occlusions in a planar or 3-dimensional object, knowing thermal, electrical, or magnetic measurements on the boundary. These defaults can be expressed as a lack of harmonicity of the solution to the associated Dirichlet-Neumann problem, thereby posing an inverse potential problem in order to recover them. In 2-D, finding an optimal discretization of the potential in Sobolev norm amounts to solve a best rational approximation problem, and the question arises as to how the location of the singularities of the approximant (*i.e.* its poles) reflects the location of the singularities of the potential (*i.e.* the defaults we seek). This is a fairly deep issue in approximation theory, to which Apics contributed convergence results for certain classes of fields expressed as Cauchy integrals over extremal contours for the logarithmic potential [39], [53] [6]. Initial schemes to locate cracks or sources *via* rational approximation on planar domains were obtained this way [56], [43], [46]. It is remarkable that finite inverse source problems in 3-D balls, or more general algebraic surfaces, can be approached using these 2-D techniques upon slicing the domain into planar sections [3], [9]. This bottom line generates a steady research activity within Apics, and again applications are sought to medical imaging and geosciences, see Sections 4.2 , 4.3 and 6.1 .

Conjectures can be raised on the behavior of optimal potential discretization in 3-D, but answering them is an ambitious program still in its infancy.

3.2.2. Systems, transfer and scattering

Participants: Laurent Baratchart, Matthias Caenepeel, Sylvain Chevillard, Sanda Lefteriu, Martine Olivi, Fabien Seyfert.

Through contacts with CNES (French space agency), members of the team became involved in identification and tuning of microwave electromagnetic filters used in space telecommunications, see Section 4.5 . The initial problem was to recover, from band-limited frequency measurements, physical parameters of the device under examination. The latter consists of interconnected dual-mode resonant cavities with negligible loss, hence its scattering matrix is modeled by a 2×2 unitary-valued matrix function on the frequency line, say the imaginary axis to fix ideas. In the bandwidth around the resonant frequency, a modal approximation of the Helmholtz equation in the cavities shows that this matrix is approximately rational, of Mc-Millan degree twice the number of cavities.

This is where system theory comes into play, through the so-called *realization* process mapping a rational transfer function in the frequency domain to a state-space representation of the underlying system of linear differential equations in the time domain. Specifically, realizing the scattering matrix allows one to construct a virtual electrical network, equivalent to the filter, the parameters of which mediate in between the frequency response and the geometric characteristics of the cavities (*i.e.* the tuning parameters).

Hardy spaces provide a framework to transform this ill-posed issue into a series of regularized analytic and meromorphic approximation problems. More precisely, the procedure sketched in Section 3.1 goes as follows:

1. infer from the pointwise boundary data in the bandwidth a stable transfer function (*i.e.* one which is holomorphic in the right half-plane), that may be infinite dimensional (numerically: of high degree). This is done by solving a problem analogous to (P) in Section 3.3.1 , while taking into account prior knowledge on the decay of the response outside the bandwidth, see [13] for details.
2. A stable rational approximation of appropriate degree to the model obtained in the previous step is performed. For this, a descent method on the compact manifold of inner matrices of given size and degree is used, based on an original parametrization of stable transfer functions developed within the team [13].
3. Realizations of this rational approximant are computed. To be useful, they must satisfy certain constraints imposed by the geometry of the device. These constraints typically come from the coupling topology of the equivalent electrical network used to model the filter. This network is composed of resonators, coupled according to some specific graph. This realization step can be recast, under appropriate compatibility conditions [8], as solving a zero-dimensional multivariate polynomial system. To tackle this problem in practice, we use Gröbner basis techniques and continuation methods which team up in the Dedale-HF software (see Section 5.4).

Let us mention that extensions of classical coupling matrix theory to frequency-dependent (reactive) couplings have lately been carried-out [1] for wide-band design applications, although further study is needed to make them computationally effective.

Subsequently Apics started to investigate issues pertaining to design rather than identification. Given the topology of the filter, a basic problem in this connection is to find the optimal response subject to specifications that bear on rejection, transmission and group delay of the scattering parameters. Generalizing the classical approach based on Chebyshev polynomials for single band filters, we recast the problem of multi-band response synthesis as a generalization of the classical Zolotarev min-max problem for rational functions [29] [11]. Thanks to quasi-convexity, the latter can be solved efficiently using iterative methods relying on linear programming. These were implemented in the software easy-FF (see Section 5.5). Currently, the team is engaged in synthesis of more complex microwave devices like multiplexers and routers, which connect several filters through wave guides. Schur analysis plays an important role here, because scattering matrices of passive systems are of Schur type (*i.e.* contractive in the stability region). The theory originates with the work of I. Schur [77], who devised a recursive test to check for contractivity of a holomorphic function in the disk. The so-called Schur parameters of a function may be viewed as Taylor coefficients for the hyperbolic metric of the disk, and the fact that Schur functions are contractions for that metric lies at the root of Schur's test. Generalizations thereof turn out to be efficient to parametrize solutions to contractive interpolation problems [31]. Dwelling on this, Apics contributed differential parametrizations (atlases of charts) of lossless matrix functions [30][12], [10] which are fundamental to our rational approximation software RARL2 (see Section 5.1). Schur analysis is also instrumental to approach de-embedding issues, and provides one with considerable insight into the so-called matching problem. The latter consists in maximizing the power a multiport can pass to a given load, and for reasons of efficiency it is all-pervasive in microwave and electric network design, *e.g.* of antennas, multiplexers, wifi cards and more. It can be viewed as a rational approximation problem in the hyperbolic metric, and the team presently gets to grips with this hot topic using multipoint contractive interpolation in the framework of the (defense funded) ANR COCORAM, see Sections 6.3.1 and 8.2.1 .

In recent years, our attention was driven by CNES and UPV (Bilbao) to questions about stability of high-frequency amplifiers, see Section 7.2 . Contrary to previously discussed devices, these are *active* components. The response of an amplifier can be linearized around a set of primary current and voltages, and then admittances of the corresponding electrical network can be computed at various frequencies, using the so-called harmonic balance method. The initial goal is to check for stability of the linearized model, so as to ascertain existence of a well-defined working state. The network is composed of lumped electrical elements namely inductors, capacitors, negative *and* positive reactors, transmission lines, and controlled current sources. Our research so far focuses on describing the algebraic structure of admittance functions, so as to set up a function-theoretic framework where the two-steps approach outlined in Section 3.1 can be put to work. The main discovery so far is that the unstable part of each partial transfer function is rational, see Section 6.4 .

3.3. Approximation

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3.3.1. Best analytic approximation

In dimension 2, the prototypical problem to be solved in step 1 of Section 3.1 may be described as: given a domain $D \subset \mathbb{R}^2$, to recover a holomorphic function from its values on a subset K of the boundary of D. For the discussion it is convenient to normalize D, which can be done by conformal mapping. So, in the simply connected case, we fix D to be the unit disk with boundary unit circle T. We denote by H^p the Hardy space of exponent p, which is the closure of polynomials in $L^p(T)$-norm if $1 \le p < \infty$ and the space of bounded holomorphic functions in D if $p = \infty$. Functions in H^p have well-defined boundary values in $L^p(T)$, which makes it possible to speak of (traces of) analytic functions on the boundary.

To find an analytic function g in D matching some measured values f approximately on a sub-arc K of T, we formulate a constrained best approximation problem as follows.

> (P) Let $1 \le p \le \infty$, K a sub-arc of T, $f \in L^p(K)$, $\psi \in L^p(T \setminus K)$ and $M > 0$; find a function $g \in H^p$ such that $\|g - \psi\|_{L^p(T \setminus K)} \le M$ and $g - f$ is of minimal norm in $L^p(K)$ under this constraint.

Here ψ is a reference behavior capturing *a priori* assumptions on the behavior of the model off K, while M is some admissible deviation thereof. The value of p reflects the type of stability which is sought and how much one wants to smooth out the data. The choice of L^p classes is suited to handle point-wise measurements.

To fix terminology, we refer to (P) as a *bounded extremal problem*. As shown in [42], [44], [50], the solution to this convex infinite-dimensional optimization problem can be obtained when $p \neq 1$ upon iterating with respect to a Lagrange parameter the solution to spectral equations for appropriate Hankel and Toeplitz operators. These spectral equations involve the solution to the special case $K = T$ of (P), which is a standard extremal problem [66]:

> (P_0) Let $1 \leq p \leq \infty$ and $\varphi \in L^p(T)$; find a function $g \in H^p$ such that $g - \varphi$ is of minimal norm in $L^p(T)$.

The case $p = 1$ is more or less open.

Various modifications of (P) can be set up in order to meet specific needs. For instance when dealing with lossless transfer functions (see Section 4.5), one may want to express the constraint on $T \setminus K$ in a point-wise manner: $|g - \psi| \leq M$ a.e. on $T \setminus K$, see [45]. In this form, the problem comes close to (but still is different from) H^∞ frequency optimization used in control [68], [76]. One can also impose bounds on the real or imaginary part of $g - \psi$ on $T \setminus K$, which is useful when considering Dirichlet-Neuman problems, see [70].

The analog of Problem (P) on an annulus, K being now the outer boundary, can be seen as a means to regularize a classical inverse problem occurring in nondestructive control, namely to recover a harmonic function on the inner boundary from Dirichlet-Neumann data on the outer boundary (see Sections 3.2.1 , 4.2 , 6.1.1 , 6.2). It may serve as a tool to approach Bernoulli type problems, where we are given data on the outer boundary and we *seek the inner boundary*, knowing it is a level curve of the solution.. In this case, the Lagrange parameter indicates how to deform the inner contour in order to improve data fitting. Similar topics are discussed in Sections 3.2.1 and 6.2 for more general equations than the Laplacian, namely isotropic conductivity equations of the form $\mathrm{div}(\sigma \nabla u) = 0$ where σ is no longer constant. Then, the Hardy spaces in Problem (P) are those of a so-called conjugate Beltrami equation: $\overline{\partial} f = \nu \overline{\partial f}$ [69], which are studied for $1 < p < \infty$ in [14], [4], [61] and [34]. Expansions of solutions needed to constructively handle such issues in the specific case of linear fractional conductivities (these occur in plasma shaping) have been expounded in [63].

Though originally considered in dimension 2, Problem (P) carries over naturally to higher dimensions where analytic functions get replaced by gradients of harmonic functions. Namely, given some open set $\Omega \subset \mathbb{R}^n$ and some $\mathbb{R}^n$-valued vector field V on an open subset O of the boundary of Ω, we seek a harmonic function in Ω whose gradient is close to V on O.

When Ω is a ball or a half-space, a substitute for holomorphic Hardy spaces is provided by the Stein-Weiss Hardy spaces of harmonic gradients [80]. Conformal maps are no longer available when $n > 2$, so that Ω can no longer be normalized. More general geometries than spheres and half-spaces have not been much studied so far.

On the ball, the analog of Problem (P) is

> (P_1) Let $1 \leq p \leq \infty$ and $B \subset \mathbb{R}^n$ the unit ball. Fix O an open subset of the unit sphere $S \subset \mathbb{R}^n$. Let further $V \in L^p(O)$ and $W \in L^p(S \setminus O)$ be $\mathbb{R}^n$-valued vector fields. Given $M > 0$, find a harmonic gradient $G \in H^p(B)$ such that $\|G - W\|_{L^p(S \setminus O)} \leq M$ and $G - V$ is of minimal norm in $L^p(O)$ under this constraint.

When $p = 2$, Problem (P_1) was solved in [2] as well as its analog on a shell. The solution extends the one given in [42] for the 2-D case, using a generalization of Toeplitz operators. Thecas of the shell was motivated An important ingredient is a refinement of the Hodge decomposition, that we call the *Hardy-Hodge* decomposition, allowing us to express a $\mathbb{R}^n$-valued vector field in $L^p(S)$, $1 < p < \infty$, as the sum of a vector field in $H^p(B)$, a vector field in $H^p(\mathbb{R}^n \setminus \overline{B})$, and a tangential divergence free vector field on S; the space of such fields is denoted by $D(S)$. If $p = 1$ or $p = \infty$, L^p must be replaced by the real Hardy space or the space of functions with bounded mean oscillation. More generally this decomposition, which is valid on any sufficiently smooth surface (see Section 6.1), seems to play a fundamental role in inverse potential problems. In fact, it was first introduced formally on the plane to describe silent magnetizations supported in $\mathbb{R}^2$ (*i.e.* those generating no field in the upper half space) [38].

Just like solving problem (P) appeals to the solution of problem (P_0), our ability to solve problem (P_1) will depend on the possibility to tackle the special case where $O = S$:

(P_2) Let $1 \le p \le \infty$ and $V \in L^p(S)$ be a $\mathbb{R}^n$-valued vector field. Find a harmonic gradient $G \in H^p(B)$ such that $\|G - V\|_{L^p(S)}$ is minimum.

Problem (P_2) is simple when $p = 2$ by virtue of the Hardy Hodge decomposition together with orthogonality of $H^2(B)$ and $H^2(\mathbb{R}^n \setminus \overline{B})$, which is the reason why we were able to solve (P_1) in this case. Other values of p cannot be treated as easily and are currently investigated by Apics, especially the case $p = \infty$ which is of particular interest and presents itself as a 3-D analog to the Nehari problem [75].

Companion to problem (P_2) is problem (P_3) below.

(P_3) Let $1 \le p \le \infty$ and $V \in L^p(S)$ be a $\mathbb{R}^n$-valued vector field. Find $G \in H^p(B)$ and $D \in D(S)$ such that $\|G + D - V\|_{L^p(S)}$ is minimum.

Note that (P_2) and (P_3) are identical in 2-D, since no non-constant tangential divergence-free vector field exists on T. It is no longer so in higher dimension, where both (P_2) and (P_3) arise in connection with source recovery in electro/magneto encephalography and paleomagnetism, see Sections 3.2.1 and 4.2 .

3.3.2. Best meromorphic and rational approximation

The techniques set forth in this section are used to solve step 2 in Section 3.2 and instrumental to approach inverse boundary value problems for the Poisson equation $\Delta u = \mu$, where μ is some (unknown) distribution.

3.3.2.1. Scalar meromorphic and rational approximation

We put R_N for the set of rational functions with at most N poles in D. By definition, meromorphic functions in $L^p(T)$ are (traces of) functions in $H^p + R_N$.

A natural generalization of problem (P_0) is:

(P_N) Let $1 \le p \le \infty$, $N \ge 0$ an integer, and $f \in L^p(T)$; find a function $g_N \in H^p + R_N$ such that $g_N - f$ is of minimal norm in $L^p(T)$.

Only for $p = \infty$ and f continuous is it known how to solve (P_N) in closed form. The unique solution is given by AAK theory (named after Adamjan, Arov and Krein), which connects the spectral decomposition of Hankel operators with best approximation [75].

The case where $p = 2$ is of special importance for it reduces to rational approximation. Indeed, if we write the Hardy decomposition $f = f^+ + f^-$ where $f^+ \in H^2$ and $f^- \in H^2(\mathbb{C} \setminus \overline{D})$, then $g_N = f^+ + r_N$ where r_N is a best approximant to f^- from R_N in $L^2(T)$. Moreover, r_N has no pole outside D, hence it is a *stable* rational approximant to f^-. However, in contrast to the case where $p = \infty$, this best approximant may *not* be unique.

The former Miaou project (predecessor of Apics) designed a dedicated steepest-descent algorithm for the case $p = 2$ whose convergence to a *local minimum* is guaranteed; until now it seems to be the only procedure meeting this property. This gradient algorithm proceeds recursively with respect to N on a compactification of the parameter space [35]. Although it has proved to be effective in all applications carried out so far (see Sections 4.2 , 4.5), it is still unknown whether the absolute minimum can always be obtained by choosing initial conditions corresponding to *critical points* of lower degree (as is done by the RARL2 software, Section 5.1).

In order to establish global convergence results, Apics has undertaken a deeper study of the number and nature of critical points (local minima, saddle points...), in which tools from differential topology and operator theory team up with classical interpolation theory [47], [49]. Based on this work, uniqueness or asymptotic uniqueness of the approximant was proved for certain classes of functions like transfer functions of relaxation systems (*i.e.* Markov functions) [51] and more generally Cauchy integrals over hyperbolic geodesic arcs [54]. These are the only results of this kind. Research by Apics on this topic remained dormant for a while by reasons of opportunity, but revisiting the work [32] in higher dimension is still a worthy endeavor. Meanwhile, an analog to AAK theory was carried out for $2 \leq p < \infty$ in [50]. Although not as effective computationally, it was recently used to derive lower bounds [26]. When $1 \leq p < 2$, problem (P_N) is still quite open.

A common feature to the above-mentioned problems is that critical point equations yield non-Hermitian orthogonality relations for the denominator of the approximant. This stresses connections with interpolation, which is a standard way to build approximants, and in many respects best or near-best rational approximation may be regarded as a clever manner to pick interpolation points. This was exploited in [55], [52], and is used in an essential manner to assess the behavior of poles of best approximants to functions with branched singularities, which is of particular interest for inverse source problems (*cf.* Sections 5.6 and 6.1).

In higher dimensions, the analog of Problem (P_N) is best approximation of a vector field by gradients of discrete potentials generated by N point masses. This basic issue is by no means fully understood, and it is an exciting research prospect. It is connected with certain generalizations of Toeplitz or Hankel operators, and with constructive approaches to so-called weak factorizations for real Hardy functions [62].

Besides, certain constrained rational approximation problems, of special interest in identification and design of passive systems, arise when putting additional requirements on the approximant, for instance that it should be smaller than 1 in modulus (*i.e.* a Schur function). In particular, Schur interpolation lately received renewed attention from the team, in connection with matching problems. There, interpolation data are subject to a well-known compatibility condition (positive definiteness of the so-called Pick matrix), and the main difficulty is to put interpolation points on the boundary of D while controlling both the degree and the extremal points of the interpolant. Results obtained by Apics in this direction generalize a variant of contractive interpolation with degree constraint studied in [67], see Section 6.3.1 . We mention that contractive interpolation with nodes approaching the boundary has been a subsidiary research topic by the team in the past, which plays an interesting role in the spectral representation of certain non-stationary stochastic processes [40], [37]. The subject is intimately connected to orthogonal polynomials on the unit circle, and this line of investigation has recently evolved towards an asymptotic study of orthogonal polynomials on planar domains, which is an active area in approximation theory with application to quantum particle systems and Hele-Shaw flows. Section 6.5.1
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3.3.2.2. Matrix-valued rational approximation

Matrix-valued approximation is necessary to handle systems with several inputs and outputs but it generates additional difficulties as compared to scalar-valued approximation, both theoretically and algorithmically. In the matrix case, the McMillan degree (*i.e.* the degree of a minimal realization in the System-Theoretic sense) generalizes the usual notion of degree for rational functions.

The basic problem that we consider now goes as follows: *let $\mathcal{F} \in (H^2)^{m\times l}$ and n an integer; find a rational matrix of size $m \times l$ without poles in the unit disk and of McMillan degree at most n which is nearest possible to $\mathcal{F}$ in $(H^2)^{m\times l}$*. Here the L^2 norm of a matrix is the square root of the sum of the squares of the norms of its entries.

The scalar approximation algorithm derived in [35] and mentioned in Section 3.3.2.1 generalizes to the matrix-valued situation [65]. The first difficulty here is to parametrize inner matrices (*i.e.* matrix-valued functions analytic in the unit disk and unitary on the unit circle) of given McMillan degree degree n. Indeed, inner matrices play the role of denominators in fractional representations of transfer matrices (using the so-called Douglas-Shapiro-Shields factorization). The set of inner matrices of given degree is a smooth manifold that allows one to use differential tools as in the scalar case. In practice, one has to produce an atlas of charts (local parametrizations) and to handle changes of charts in the course of the algorithm. Such parametrization can be obtained using interpolation theory and Schur-type algorithms, the parameters of which are vectors or matrices ([30], [10], [12]). Some of these parametrizations are also interesting to compute realizations and achieve filter synthesis ([10] [12]). The rational approximation software “RARL2” developed by the team is described in Section 5.1 .

Difficulties relative to multiple local minima of course arise in the matrix-valued case as well, and deriving criteria that guarantee uniqueness is even more difficult than in the scalar case. The case of rational functions of degree n or small perturbations thereof (the consistency problem) was solved in [48]. Matrix-valued Markov functions are the only known example beyond this one [33].

Let us stress that RARL2 seems the only algorithm handling rational approximation in the matrix case that demonstrably converges to a local minimum while meeting stability constraints on the approximant.

3.3.3. Behavior of poles of meromorphic approximants

Participant: Laurent Baratchart.

We refer here to the behavior of poles of best meromorphic approximants, in the L^p-sense on a closed curve, to functions f defined as Cauchy integrals of complex measures whose support lies inside the curve. Normalizing the contour to be the unit circle T, we are back to Problem (P_N) in Section 3.3.2.1 ; invariance of the latter under conformal mapping was established in [5]. Research so far has focused on functions whose singular set inside the contour is zero or one-dimensional.

Generally speaking in approximation theory, assessing the behavior of poles of rational approximants is essential to obtain error rates as the degree goes large, and to tackle constructive issues like uniqueness. However, as explained in Section 3.2.1 , Apics considers this issue foremost as a means to extract information on singularities of the solution to a Dirichlet-Neumann problem. The general theme is thus: *how do the singularities of the approximant reflect those of the approximated function?* This approach to inverse problem for the 2-D Laplacian turns out to be attractive when singularities are zero- or one-dimensional (see Section 4.2). It can be used as a computationally cheap initial condition for more precise but much heavier numerical optimizations which often do not even converge unless properly initialized. As regards crack detection or source recovery, this approach boils down to analyzing the behavior of best meromorphic approximants of a function with branch points. For piecewise analytic cracks, or in the case of sources, we were able to prove ([5], [6], [39]), that the poles of the approximants accumulate, when the degree goes large, to some extremal cut of minimum weighted logarithmic capacity connecting the singular points of the crack, or the sources [43]. Moreover, the asymptotic density of the poles turns out to be the Green equilibrium distribution on this cut in D, therefore it charges the singular points if one is able to approximate in sufficiently high degree (this is where the method could fail, because high-order approximation requires rather precise data).

The case of two-dimensional singularities is still an outstanding open problem.

It is remarkable that inverse source problems inside a sphere or an ellipsoid in 3-D can be approached with such 2-D techniques, as applied to planar sections (see Section 6.1). The technique is implemented in the software FindSources3D, see Section 5.6 .

3.3.4. Miscellaneous

Participant: Sylvain Chevillard.

Sylvain Chevillard, joined team in November 2010. His coming resulted in Apics hosting a research activity in certified computing, centered on the software *Sollya* of which S. Chevillard is a co-author, see Section 5.7 . On the one hand, Sollya is an Inria software which still requires some tuning to a growing community of users. On the other hand, approximation-theoretic methods at work in Sollya are potentially useful for certified solutions to constrained analytic problems described in Section 3.3.1 . However, developing Sollya is not a long-term objective of Apics.

BIPOP Project-Team

3. Research Program

3.1. Dynamic non-regular systems

mechanical systems, impacts, unilateral constraints, complementarity, modeling, analysis, simulation, control, convex analysis

Dynamical systems (we limit ourselves to finite-dimensional ones) are said to be *non-regular* whenever some nonsmoothness of the state arises. This nonsmoothness may have various roots: for example some outer impulse, entailing so-called *differential equations with measure*. An important class of such systems can be described by the complementarity system

$$\begin{cases} \dot{x} = f(x, u, \lambda)\,, \\ 0 \leq y \perp \lambda \geq 0\,, \\ g(y, \lambda, x, u, t) = 0\,, \\ \text{re-initialization law of the state } x(\cdot)\,, \end{cases} \tag{20}$$

where $\perp$ denotes orthogonality; u is a control input. Now (1) can be viewed from different angles.

- Hybrid systems: it is in fact natural to consider that (1) corresponds to different models, depending whether $y_i = 0$ or $y_i > 0$ (y_i being a component of the vector y). In some cases, passing from one mode to the other implies a jump in the state x; then the continuous dynamics in (1) may contain distributions.
- Differential inclusions: $0 \leq y \perp \lambda \geq 0$ is equivalent to $-\lambda \in \mathrm{N}_K(y)$, where K is the nonnegative orthant and $\mathrm{N}_K(y)$ denotes the normal cone to K at y. Then it is not difficult to reformulate (1) as a differential inclusion.
- Dynamic variational inequalities: such a formalism reads as $\langle \dot{x}(t) + F(x(t), t), v - x(t) \rangle \geq 0$ for all $v \in K$ and $x(t) \in K$, where K is a nonempty closed convex set. When K is a polyhedron, then this can also be written as a complementarity system as in (1).

Thus, the 2nd and 3rd lines in (1) define the modes of the hybrid systems, as well as the conditions under which transitions occur from one mode to another. The 4th line defines how transitions are performed by the state x. There are several other formalisms which are quite related to complementarity. A tutorial-survey paper has been published [5], whose aim is to introduce the dynamics of complementarity systems and the main available results in the fields of mathematical analysis, analysis for control (controllability, observability, stability), and feedback control.

3.2. Nonsmooth optimization

optimization, numerical algorithm, convexity, Lagrangian relaxation, combinatorial optimization.

Here we are dealing with the minimization of a function f (say over the whole space R^n), whose derivatives are discontinuous. A typical situation is when f comes from dualization, if the primal problem is not strictly convex – for example a large-scale linear program – or even nonconvex – for example a combinatorial optimization problem. Also important is the case of spectral functions, where $f(x) = F(\lambda(A(x)))$, A being a symmetric matrix and λ its spectrum.

For these types of problems, we are mainly interested in developing efficient resolution algorithms. Our basic tool is bundling (Chap. XV of [11]) and we act along two directions:

- To explore application areas where nonsmooth optimization algorithms can be applied, possibly after some tayloring. A rich field of such application is combinatorial optimization, with all forms of relaxation [12].
- To explore the possibility of designing more sophisticated algorithms. This implies an appropriate generalization of second derivatives when the first derivative does not exist, and we use advanced tools of nonsmooth analysis, for example [14].

COMMANDS Project-Team

3. Research Program

3.1. Historical aspects

The roots of deterministic optimal control are the "classical" theory of the calculus of variations, illustrated by the work of Newton, Bernoulli, Euler, and Lagrange (whose famous multipliers were introduced in [84]), with improvements due to the "Chicago school", Bliss [51] during the first part of the 20th century, and by the notion of relaxed problem and generalized solution (Young [93]).

Trajectory optimization really started with the spectacular achievement done by Pontryagin's group [90] during the fifties, by stating, for general optimal control problems, nonlocal optimality conditions generalizing those of Weierstrass. This motivated the application to many industrial problems (see the classical books by Bryson and Ho [59], Leitmann [86], Lee and Markus [85], Ioffe and Tihomirov [76]). Since then, various theoretical achievements have been obtained by extending the results to nonsmooth problems, see Aubin [47], Clarke [60], Ekeland [67].

Dynamic programming was introduced and systematically studied by R. Bellman during the fifties. The HJB equation, whose solution is the value function of the (parameterized) optimal control problem, is a variant of the classical Hamilton-Jacobi equation of mechanics for the case of dynamics parameterized by a control variable. It may be viewed as a differential form of the dynamic programming principle. This nonlinear first-order PDE appears to be well-posed in the framework of *viscosity solutions* introduced by Crandall and Lions [62], [63], [61]. These tools also allow to perform the numerical analysis of discretization schemes. The theoretical contributions in this direction did not cease growing, see the books by Barles [49] and Bardi and Capuzzo-Dolcetta [48].

3.2. Trajectory optimization

The so-called *direct methods* consist in an optimization of the trajectory, after having discretized time, by a nonlinear programming solver that possibly takes into account the dynamic structure. So the two main problems are the choice of the discretization and the nonlinear programming algorithm. A third problem is the possibility of refinement of the discretization once after solving on a coarser grid.

In the *full discretization approach*, general Runge-Kutta schemes with different values of control for each inner step are used. This allows to obtain and control high orders of precision, see Hager [73], Bonnans [54]. In an interior-point algorithm context, controls can be eliminated and the resulting system of equation is easily solved due to its band structure. Discretization errors due to constraints are discussed in Dontchev et al. [66]. See also Malanowski et al. [87].

In the *indirect* approach, the control is eliminated thanks to Pontryagin's maximum principle. One has then to solve the two-points boundary value problem (with differential variables state and costate) by a single or multiple shooting method. The questions are here the choice of a discretization scheme for the integration of the boundary value problem, of a (possibly globalized) Newton type algorithm for solving the resulting finite dimensional problem in IR^n (n is the number of state variables), and a methodology for finding an initial point.

For state constrained problems or singular arcs, the formulation of the shooting function may be quite elaborate [52], [53], [46]. As initiated in [70], we focus more specifically on the handling of discontinuities, with ongoing work on the geometric integration aspects (Hamiltonian conservation).

3.3. Hamilton-Jacobi-Bellman approach

This approach consists in calculating the value function associated with the optimal control problem, and then synthesizing the feedback control and the optimal trajectory using Pontryagin's principle. The method has the great particular advantage of reaching directly the global optimum, which can be very interesting when the problem is not convex.

Characterization of the value function >From the dynamic programming principle, we derive a characterization of the value function as being a solution (in viscosity sense) of an Hamilton-Jacobi-Bellman equation, which is a nonlinear PDE of dimension equal to the number n of state variables. Since the pioneer works of Crandall and Lions [62], [63], [61], many theoretical contributions were carried out, allowing an understanding of the properties of the value function as well as of the set of admissible trajectories. However, there remains an important effort to provide for the development of effective and adapted numerical tools, mainly because of numerical complexity (complexity is exponential with respect to n).

Numerical approximation for continuous value function Several numerical schemes have been already studied to treat the case when the solution of the HJB equation (the value function) is continuous. Let us quote for example the Semi-Lagrangian methods [69], [68] studied by the team of M. Falcone (La Sapienza, Rome), the high order schemes WENO, ENO, Discrete galerkin introduced by S. Osher, C.-W. Shu, E. Harten [74], [75], [75], [88], and also the schemes on nonregular grids by R. Abgrall [45], [44]. All these schemes rely on finite differences or/and interpolation techniques which lead to numerical diffusions. Hence, the numerical solution is unsatisfying for long time approximations even in the continuous case.

One of the (nonmonotone) schemes for solving the HJB equation is based on the Ultrabee algorithm proposed, in the case of advection equation with constant velocity, by Roe [92] and recently revisited by Després-Lagoutière [65], [64]. The numerical results on several academic problems show the relevance of the antidiffusive schemes. However, the theoretical study of the convergence is a difficult question and is only partially done.

Optimal stochastic control problems occur when the dynamical system is uncertain. A decision typically has to be taken at each time, while realizations of future events are unknown (but some information is given on their distribution of probabilities). In particular, problems of economic nature deal with large uncertainties (on prices, production and demand). Specific examples are the portfolio selection problems in a market with risky and non-risky assets, super-replication with uncertain volatility, management of power resources (dams, gas). Air traffic control is another example of such problems.

Nonsmoothness of the value function. Sometimes the value function is smooth (e.g. in the case of Merton's portfolio problem, Oksendal [94]) and the associated HJB equation can be solved explicitly. Still, the value function is not smooth enough to satisfy the HJB equation in the classical sense. As for the deterministic case, the notion of viscosity solution provides a convenient framework for dealing with the lack of smoothness, see Pham [89], that happens also to be well adapted to the study of discretization errors for numerical discretization schemes [77], [50].

Numerical approximation for optimal stochastic control problems. The numerical discretization of second order HJB equations was the subject of several contributions. The book of Kushner-Dupuis [83] gives a complete synthesis on the Markov chain schemes (i.e Finite Differences, semi-Lagrangian, Finite Elements, ...). Here a main difficulty of these equations comes from the fact that the second order operator (i.e. the diffusion term) is not uniformly elliptic and can be degenerated. Moreover, the diffusion term (covariance matrix) may change direction at any space point and at any time (this matrix is associated the dynamics volatility).

For solving stochastic control problems, we studied the so-called Generalized Finite Differences (GFD), that allow to choose at any node, the stencil approximating the diffusion matrix up to a certain threshold [57]. Determining the stencil and the associated coefficients boils down to a quadratic program to be solved at each point of the grid, and for each control. This is definitely expensive, with the exception of special structures where the coefficients can be computed at low cost. For two dimensional systems, we designed a (very) fast algorithm for computing the coefficients of the GFD scheme, based on the Stern-Brocot tree [56].

CORIDA Team

3. Research Program

3.1. Analysis and control of fluids and of fluid-structure interactions

Participants: Thomas Chambrion, Antoine Henrot, Alexandre Munnier, Lionel Rosier, Jean-François Scheid, Takéo Takahashi, Marius Tucsnak, Jean-Claude Vivalda.

The problems we consider are modeled by the Navier-Stokes, Euler or Korteweg de Vries equations (for the fluid) coupled to the equations governing the motion of the solids. One of the main difficulties of this problem comes from the fact that the domain occupied by the fluid is one of the unknowns of the problem. We have thus to tackle a *free boundary problem*.

The control of fluid flows is a major challenge in many applications: aeronautics, pollution issues, regulation of irrigation channels or of the flow in pipelines, etc. All these problems cannot be easily reduced to finite dimensional models so a methodology of analysis and control based on PDE's is an essential issue. In a first approximation the motion of fluid and of the solids can be decoupled. The most used models for an incompressible fluid are given by the Navier-Stokes or by the Euler equations.

The optimal open loop control approach of these models has been developed from both the theoretical and numerical points of view. Controllability issues for the equations modeling the fluid motion are by now well understood (see, for instance, Imanuvilov [52] and the references therein). The feedback control of fluid motion has also been recently investigated by several research teams (see, for instance Barbu [47] and references therein) but this field still contains an important number of open problems (in particular those concerning observers and implementation issues). One of our aims is to develop efficient tools for computing feedback laws for the control of fluid systems.

In real applications the fluid is often surrounded by or it surrounds an elastic structure. In the above situation one has to study fluid-structure interactions. This subject has been intensively studied during the last years, in particular for its applications in noise reduction problems, in lubrication issues or in aeronautics. In this kind of problems, a PDE's system modeling the fluid in a cavity (Laplace equation, wave equation, Stokes, Navier-Stokes or Euler systems) is coupled to the equations modeling the motion of a part of the boundary. The difficulties of this problem are due to several reasons such as the strong nonlinear coupling and the existence of a free boundary. This partially explains the fact that applied mathematicians have only recently tackled these problems from either the numerical or theoretical point of view. One of the main results obtained in our project concerns the global existence of weak solutions in the case of a two-dimensional Navier–Stokes fluid [59]. Another important result gives the existence and the uniqueness of strong solutions for two or three-dimensional Navier–Stokes fluid [61]. In that case, the solution exists as long as there is no contact between rigid bodies, and for small data in the three-dimensional case.

3.2. Frequency domain methods for the analysis and control of systems governed by PDE's

Participants: Xavier Antoine, Bruno Pinçon, Karim Ramdani.

We use frequency tools to analyze different types of problems. The first one concerns the control, the optimal control and the stabilization of systems governed by PDE's, and their numerical approximations. The second one concerns time-reversal phenomena, while the last one deals with numerical approximation of high-frequency scattering problems.

3.2.1. Control and stabilization for skew-adjoint systems

The first area concerns theoretical and numerical aspects in the control of a class of PDE's. More precisely, in a semigroup setting, the systems we consider have a skew-adjoint generator. Classical examples are the wave, the Bernoulli-Euler or the Schrödinger equations. Our approach is based on an original characterization of exact controllability of second order conservative systems proposed by K. Liu [56]. This characterization can be related to the Hautus criterion in the theory of finite dimensional systems (cf. [51]). It provides for time-dependent problems exact controllability criteria *that do not depend on time, but depend on the frequency variable* conjugated to time. Studying the controllability of a given system amounts then to establishing uniform (with respect to frequency) estimates. In other words, the problem of exact controllability for the wave equation, for instance, comes down to a high-frequency analysis for the Helmholtz operator. This frequency approach has been proposed first by K. Liu for bounded control operators (corresponding to internal control problems), and has been recently extended to the case of unbounded control operators (and thus including boundary control problems) by L. Miller [57]. Using the result of Miller, K. Ramdani, T. Takahashi, M. Tucsnak have obtained in [5] a new spectral formulation of the criterion of Liu [56], which is valid for boundary control problems. This frequency test can be seen as an observability condition for packets of eigenvectors of the operator. This frequency test has been successfully applied in [5] to study the exact controllability of the Schrödinger equation, the plate equation and the wave equation in a square. Let us emphasize here that one further important advantage of this frequency approach lies in the fact that it can also be used for the analysis of space semi-discretized control problems (by finite element or finite differences). The estimates to be proved must then be uniform with respect to *both the frequency and the mesh size*.

In the case of finite dimensional systems one of the main applications of frequency domain methods consists in designing robust controllers, in particular of H^∞ type. Obtaining the similar tools for systems governed by PDE's is one of the major challenges in the theory of infinite dimensional systems. The first difficulty which has to be tackled is that, even for very simple PDE systems, no method giving the parametrisation of all stabilizing controllers is available. One of the possible remedies consists in considering known families of stabilizing feedback laws depending on several parameters and in optimizing the H^∞ norm of an appropriate transfer function with respect to this parameters. Such families of feedback laws yielding computationally tractable optimization problems are now available for systems governed by PDE's in one space dimension.

3.2.2. Time-reversal

The second area in which we make use of frequency tools is the analysis of time-reversal for harmonic acoustic waves. This phenomenon described in Fink [49] is a direct consequence of the reversibility of the wave equation in a non dissipative medium. It can be used to **focus an acoustic wave** on a target through a complex and/or unknown medium. To achieve this, the procedure followed is quite simple. First, time-reversal mirrors are used to generate an incident wave that propagates through the medium. Then, the mirrors measure the acoustic field diffracted by the targets, time-reverse it and back-propagate it in the medium. Iterating the scheme, we observe that the incident wave emitted by the mirrors focuses on the scatterers. An alternative and more original focusing technique is based on the so-called D.O.R.T. method [50]. According to this experimental method, the eigenelements of the time-reversal operator contain important information on the propagation medium and on the scatterers contained in it. More precisely, the number of nonzero eigenvalues is exactly the number of scatterers, while each eigenvector corresponds to an incident wave that selectively focuses on each scatterer.

Time-reversal has many applications covering a wide range of fields, among which we can cite *medicine* (kidney stones destruction or medical imaging), *sub-marine communication* and *non destructive testing*. Let us emphasize that in the case of time-harmonic acoustic waves, time-reversal is equivalent to phase conjugation and involves the Helmholtz operator.

In [2], we proposed the first far field model of time reversal in the time-harmonic case.

3.2.3. Numerical approximation of high-frequency scattering problems

This subject deals mainly with the numerical solution of the Helmholtz or Maxwell equations for open region scattering problems. This kind of situation can be met e.g. in radar systems in electromagnetism or in acoustics for the detection of underwater objects like submarines.

Two particular difficulties are considered in this situation

- the wavelength of the incident signal is small compared to the characteristic size of the scatterer,
- the problem is set in an unbounded domain.

These two problematics limit the application range of most common numerical techniques. The aim of this part is to develop new numerical simulation techniques based on microlocal analysis for modeling the propagation of rays. The importance of microlocal techniques in this situation is that it makes possible a local analysis both in the spatial and frequency domain. Therefore, it can be seen as a kind of asymptotic theory of rays which can be combined with numerical approximation techniques like boundary element methods. The resulting method is called the On-Surface Radiation Condition method.

3.3. Observability, controllability and stabilization in the time domain

Participants: Fatiha Alabau-Boussouira, Xavier Antoine, Thomas Chambrion, Antoine Henrot, Karim Ramdani, Marius Tucsnak, Jean-Claude Vivalda.

Controllability and observability have been set at the center of control theory by the work of R. Kalman in the 1960's and soon they have been generalized to the infinite-dimensional context. The main early contributors have been D.L. Russell, H. Fattorini, T. Seidman, R. Triggiani, W. Littman and J.-L. Lions. The latter gave the field an enormous impact with his book [54], which is still a main source of inspiration for many researchers. Unlike in classical control theory, for infinite-dimensional systems there are many different (and not equivalent) concepts of controllability and observability. The strongest concepts are called exact controllability and exact observability, respectively. In the case of linear systems exact controllability is important because it guarantees stabilizability and the existence of a linear quadratic optimal control. Dually, exact observability guarantees the existence of an exponentially converging state estimator and the existence of a linear quadratic optimal filter. An important feature of infinite dimensional systems is that, unlike in the finite dimensional case, the conditions for exact observability are no longer independent of time. More precisely, for simple systems like a string equation, we have exact observability only for times which are large enough. For systems governed by other PDE's (like dispersive equations) the exact observability in arbitrarily small time has been only recently established by using new frequency domain techniques. A natural question is to estimate the energy required to drive a system in the desired final state when the control time goes to zero. This is a challenging theoretical issue which is critical for perturbation and approximation problems. In the finite dimensional case this issue has been first investigated in Seidman [60]. In the case of systems governed by linear PDE's some similar estimates have been obtained only very recently (see, for instance Miller [57]). One of the open problems of this field is to give sharp estimates of the observability constants when the control time goes to zero.

Even in the finite-dimensional case, despite the fact that the linear theory is well established, many challenging questions are still open, concerning in particular nonlinear control systems.

In some cases it is appropriate to regard external perturbations as unknown inputs; for these systems the synthesis of observers is a challenging issue, since one cannot take into account the term containing the unknown input into the equations of the observer. While the theory of observability for linear systems with unknown inputs is well established, this is far from being the case in the nonlinear case. A related active field of research is the uniform stabilization of systems with time-varying parameters. The goal in this case is to stabilize a control system with a control strategy independent of some signals appearing in the dynamics, i.e., to stabilize simultaneously a family of time-dependent control systems and to characterize families of control systems that can be simultaneously stabilized.

One of the basic questions in finite- and infinite-dimensional control theory is that of motion planning, i.e., the explicit design of a control law capable of driving a system from an initial state to a prescribed final one. Several techniques, whose suitability depends strongly on the application which is considered, have been and are being developed to tackle such a problem, as for instance the continuation method, flatness, tracking or optimal control. Preliminary to any question regarding motion planning or optimal control is the issue of controllability, which is not, in the general nonlinear case, solved by the verification of a simple algebraic criterion. A further motivation to study nonlinear controllability criteria is given by the fact that techniques developed in the domain of (finite-dimensional) geometric control theory have been recently applied successfully to study the controllability of infinite-dimensional control systems, namely the Navier–Stokes equations (see Agrachev and Sarychev [46]).

3.4. Implementation

This is a transverse research axis since all the research directions presented above have to be validated by giving control algorithms which are aimed to be implemented in real control systems. We stress below some of the main points which are common (from the implementation point of view) to the application of the different methods described in the previous sections.

For many infinite dimensional systems the use of co-located actuators and sensors and of simple proportional feed-back laws gives satisfying results. However, for a large class of systems of interest it is not clear that these feedbacks are efficient, or the use of co-located actuators and sensors is not possible. This is why a more general approach for the design of the feedbacks has to be considered. Among the techniques in finite dimensional systems theory those based on the solutions of infinite dimensional Riccati equation seem the most appropriate for a generalization to infinite dimensional systems. The classical approach is to approximate an LQR problem for a given infinite dimensional system by finite dimensional LQR problems. As it has been already pointed out in the literature this approach should be carefully analyzed since, even for some very simple examples, the sequence of feedbacks operators solving the finite dimensional LQR is not convergent. Roughly speaking this means that by refining the mesh we obtain a closed loop system which is not exponentially stable (even if the corresponding infinite dimensional system is theoretically stabilized). In order to overcome this difficulty, several methods have been proposed in the literature : filtering of high frequencies, multigrid methods or the introduction of a numerical viscosity term. We intend to first apply the numerical viscosity method introduced in Tcheougoue Tebou – Zuazua [62], for optimal and robust control problems.

DISCO Project-Team

3. Research Program

3.1. Modeling of complex environment

We want to model phenomena such as a temporary loss of connection (e.g. synchronisation of the movements through haptic interfaces), a nonhomogeneous environment (e.g. case of cryogenic systems) or the presence of the human factor in the control loop (e.g. grid systems) but also problems involved with technological constraints (e.g. range of the sensors). The mathematical models concerned include integro-differential, partial differential equations, algebraic inequalities with the presence of several time scales, whose variables and/or parameters must satisfy certain constraints (for instance, positivity).

3.2. Analysis of interconnected systems

- Algebraic analysis of linear systems

  Study of the structural properties of linear differential time-delay systems and linear infinite-dimensional systems (e.g. invariants, controllability, observability, flatness, reductions, decomposition, decoupling, equivalences) by means of constructive algebra, module theory, homological algebra, algebraic analysis and symbolic computation [8], [9], [71], [91], [72], [75].

- Robust stability of linear systems

  Within an interconnection context, lots of phenomena are modelled directly or after an approximation by delay systems. These systems might have fixed delays, time-varying delays, distributed delays ...

  For various infinite-dimensional systems, particularly delay and fractional systems, input-output and time-domain methods are jointly developed in the team to characterize stability. This research is developed at four levels: analytic approaches (H_∞-stability, BIBO-stablity, robust stability, robustness metrics) [1], [2], [5], [6], symbolic computation approaches (SOS methods are used for determining easy-to-check conditions which guarantee that the poles of a given linear system are not in the closed right half-plane, certified CAD techniques), numerical approaches (root-loci, continuation methods) and by means of softwares developed in the team [5], [6].

- Robustness/fragility of biological systems

  Deterministic biological models describing, for instance, species interactions, are frequently composed of equations with important disturbances and poorly known parameters. To evaluate the impact of the uncertainties, we use the techniques of designing of global strict Lyapunov functions or functional developed in the team.

  However, for other biological systems, the notion of robustness may be different and this question is still in its infancy (see, e.g. [83]). Unlike engineering problems where a major issue is to maintain stability in the presence of disturbances, a main issue here is to maintain the system response in the presence of disturbances. For instance, a biological network is required to keep its functioning in case of a failure of one of the nodes in the network. The team, which has a strong expertise in robustness for engineering problems, aims at contributing at the develpment of new robustness metrics in this biological context.

3.3. Stabilization of interconnected systems

- Linear systems: Analytic and algebraic approaches are considered for infinite-dimensional linear systems studied within the input-output framework.

  In the recent years, the Youla-Kučera parametrization (which gives the set of all stabilizing controllers of a system in terms of its coprime factorizations) has been the cornerstone of the success of the H_∞-control since this parametrization allows one to rewrite the problem of finding the optimal stabilizing controllers for a certain norm such as H_∞ or H_2 as affine, and thus, convex problem.

  A central issue studied in the team is the computation of such factorizations for a given infinite-dimensional linear system as well as establishing the links between stabilizability of a system for a certain norm and the existence of coprime factorizations for this system. These questions are fundamental for robust stabilization problems [1], [2], [8], [9].

  We also consider simultaneous stabilization since it plays an important role in the study of reliable stabilization, i.e. in the design of controllers which stabilize a finite family of plants describing a system during normal operating conditions and various failed modes (e.g. loss of sensors or actuators, changes in operating points) [9]. Moreover, we investigate strongly stabilizable systems [9], namely systems which can be stabilized by stable controllers, since they have a good ability to track reference inputs and, in practice, engineers are reluctant to use unstable controllers especially when the system is stable.

- Nonlinear systems

  The project aims at developing robust stabilization theory and methods for important classes of nonlinear systems that ensure good controller performance under uncertainty and time delays. The main techniques include techniques called backstepping and forwarding, contructions of strict Lyapunov functions through so-called "strictification" approaches [3] and construction of Lyapunov-Krasovskii functionals [4], [5], [6].

- Predictive control

  For highly complex systems described in the time-domain and which are submitted to constraints, predictive control seems to be well-adapted. This model based control method (MPC: Model Predictive Control) is founded on the determination of an optimal control sequence over a receding horizon. Due to its formulation in the time-domain, it is an effective tool for handling constraints and uncertainties which can be explicitly taken into account in the synthesis procedure [7]. The team considers how mutiparametric optimization can help to reduce the computational load of this method, allowing its effective use on real world constrained problems.

  The team also investigates stochastic optimization methods such as genetic algorithm, particle swarm optimization or ant colony [10] as they can be used to optimize any criterion and constraint whatever their mathematical structure is. The developed methodologies can be used by non specialists.

3.4. Synthesis of reduced complexity controllers

- PID controllers

  Even though the synthesis of control laws of a given complexity is not a new problem, it is still open, even for finite-dimensional linear systems. Our purpose is to search for good families of “simple” (e.g. low order) controllers for infinite-dimensional dynamical systems. Within our approach, PID candidates are first considered in the team [2], [87].

- Predictive control

  The synthesis of predictive control laws is concerned with the solution of multiparametric optimization problems. Reduced order controller constraints can be viewed as non convex constraints in the synthesis procedure. Such constraints can be taken into account with stochastic algorithms.

Finally, the development of algorithms based on both symbolic computation and numerical methods, and their implementations in dedicated Scilab/Matlab/Maple toolboxes are important issues in the project.

GECO Project-Team

3. Research Program

3.1. Geometric control theory

The main research topic of the project-team will be **geometric control**, with a special focus on **control design**. The application areas that we target are control of quantum mechanical systems, neurogeometry and switched systems.

Geometric control theory provides a viewpoint and several tools, issued in particular from differential geometry, to tackle typical questions arising in the control framework: controllability, observability, stabilization, optimal control... [32], [66] The geometric control approach is particularly well suited for systems involving nonlinear and nonholonomic phenomena. We recall that nonholonomicity refers to the property of a velocity constraint that is not equivalent to a state constraint.

The expression **control design** refers here to all phases of the construction of a control law, in a mainly open-loop perspective: modeling, controllability analysis, output tracking, motion planning, simultaneous control algorithms, tracking algorithms, performance comparisons for control and tracking algorithms, simulation and implementation.

We recall that

- **controllability** denotes the property of a system for which any two states can be connected by a trajectory corresponding to an admissible control law ;
- **output tracking** refers to a control strategy aiming at keeping the value of some functions of the state arbitrarily close to a prescribed time-dependent profile. A typical example is **configuration tracking** for a mechanical system, in which the controls act as forces and one prescribes the position variables along the trajectory, while the evolution of the momenta is free. One can think for instance at the lateral movement of a car-like vehicle: even if such a movement is unfeasible, it can be tracked with arbitrary precision by applying a suitable control strategy;
- **motion planning** is the expression usually denoting the algorithmic strategy for selecting one control law steering the system from a given initial state to an attainable final one;
- **simultaneous control** concerns algorithms that aim at driving the system from two different initial conditions, with the same control law and over the same time interval, towards two given final states (one can think, for instance, at some control action on a fluid whose goal is to steer simultaneously two floating bodies.) Clearly, the study of which pairs (or n-uples) of states can be simultaneously connected thanks to an admissible control requires an additional controllability analysis with respect to the plain controllability mentioned above.

At the core of control design is then the notion of motion planning. Among the motion planning methods, a preeminent role is played by those based on the Lie algebra associated with the control system ([86], [73], [79]), those exploiting the possible flatness of the system ([60]) and those based on the continuation method ([98]). Optimal control is clearly another method for choosing a control law connecting two states, although it generally introduces new computational and theoretical difficulties.

Control systems with special structure, which are very important for applications are those for which the controls appear linearly. When the controls are not bounded, this means that the admissible velocities form a distribution in the tangent bundle to the state manifold. If the distribution is equipped with a smoothly varying norm (representing a cost of the control), the resulting geometrical structure is called *sub-Riemannian*. Sub-Riemannian geometry thus appears as the underlying geometry of the nonholonomic control systems, playing the same role as Euclidean geometry for linear systems. As such, its study is fundamental for control design. Moreover its importance goes far beyond control theory and is an active field of research both in differential geometry ([85]), geometric measure theory ([61], [36]) and hypoelliptic operator theory ([48]).

Other important classes of control systems are those modeling mechanical systems. The dynamics are naturally defined on the tangent or cotangent bundle of the configuration manifold, they have Lagrangian or Hamiltonian structure, and the controls act as forces. When the controls appear linearly, the resulting model can be seen somehow as a second-order sub-Riemannian structure (see [53]).

The control design topics presented above naturally extend to the case of distributed parameter control systems. The geometric approach to control systems governed by partial differential equations is a novel subject with great potential. It could complement purely analytical and numerical approaches, thanks to its more dynamical, qualitative and intrinsic point of view. An interesting example of this approach is the paper [33] about the controllability of Navier–Stokes equation by low forcing modes.

I4S Project-Team

3. Research Program

3.1. Introduction

In this section, the main features for the key monitoring issues, namely identification, detection, and diagnostics, are provided, and a particular instantiation relevant for vibration monitoring is described.

It should be stressed that the foundations for identification, detection, and diagnostics, are fairly general, if not generic. Handling high order linear dynamical systems, in connection with finite elements models, which call for using subspace-based methods, is specific to vibration-based SHM. Actually, one particular feature of model-based sensor information data processing as exercised in I4S, is the combined use of black-box or semi-physical models together with physical ones. Black-box and semi-physical models are, for example, eigenstructure parameterizations of linear MIMO systems, of interest for modal analysis and vibration-based SHM. Such models are intended to be identifiable. However, due to the large model orders that need to be considered, the issue of model order selection is really a challenge. Traditional advanced techniques from statistics such as the various forms of Akaike criteria (AIC, BIC, MDL, ...) do not work at all. This gives rise to new research activities specific to handling high order models.

Our approach to monitoring assumes that a model of the monitored system is available. This is a reasonable assumption, especially within the SHM areas. The main feature of our monitoring method is its intrinsic ability to the early warning of small deviations of a system with respect to a reference (safe) behavior under usual operating conditions, namely without any artificial excitation or other external action. Such a normal behavior is summarized in a reference parameter vector θ_0, for example a collection of modes and mode-shapes.

3.2. Identification

The behavior of the monitored continuous system is assumed to be described by a parametric model $\{\mathbf{P}_\theta\,,\, \theta \in \Theta\}$, where the distribution of the observations $(Z_0, ..., Z_N)$ is characterized by the parameter vector $\theta \in \Theta$. An *estimating function*, for example of the form :

$$\mathcal{K}_N(\theta) = 1/N \sum_{k=0}^{N} K(\theta, Z_k)$$

is such that $\mathbf{E}_\theta[\mathcal{K}_N(\theta)] = 0$ for all $\theta \in \Theta$. In many situations, $\mathcal{K}$ is the gradient of a function to be minimized : squared prediction error, log-likelihood (up to a sign), ... For performing model identification on the basis of observations $(Z_0, ..., Z_N)$, an estimate of the unknown parameter is then [61] :

$$\widehat{\theta}_N = \arg\{\theta \in \Theta \,:\, \mathcal{K}_N(\theta) = 0\}$$

In many applications, such an approach must be improved in the following directions :

- *Recursive estimation:* the ability to compute $\widehat{\theta}_{N+1}$ simply from $\widehat{\theta}_N$;
- *Adaptive estimation:* the ability to *track* the true parameter θ^* when it is time-varying.

3.3. Detection

Our approach to on-board detection is based on the so-called asymptotic statistical local approach, which we have extended and adapted [5], [4], [2]. It is worth noticing that these investigations of ours have been initially motivated by a vibration monitoring application example. It should also be stressed that, as opposite to many monitoring approaches, our method does not require repeated identification for each newly collected data sample.

For achieving the early detection of small deviations with respect to the normal behavior, our approach generates, on the basis of the reference parameter vector θ_0 and a new data record, indicators which automatically perform :

- The early detection of a slight mismatch between the model and the data;
- A preliminary diagnostics and localization of the deviation(s);
- The tradeoff between the magnitude of the detected changes and the uncertainty resulting from the estimation error in the reference model and the measurement noise level.

These indicators are computationally cheap, and thus can be embedded. This is of particular interest in some applications, such as flutter monitoring.

As in most fault detection approaches, the key issue is to design a *residual*, which is ideally close to zero under normal operation, and has low sensitivity to noises and other nuisance perturbations, but high sensitivity to small deviations, before they develop into events to be avoided (damages, faults, ...). The originality of our approach is to :

- *Design* the residual basically as a *parameter estimating function*,
- *Evaluate* the residual thanks to a kind of central limit theorem, stating that the residual is asymptotically Gaussian and reflects the presence of a deviation in the parameter vector through a change in its own mean vector, which switches from zero in the reference situation to a non-zero value.

This is actually a strong result, which transforms any detection problem concerning a parameterized stochastic *process* into the problem of monitoring the mean of a Gaussian *vector*.

The behavior of the monitored system is again assumed to be described by a parametric model $\{\mathbf{P}_\theta \,,\, \theta \in \Theta\}$, and the safe behavior of the process is assumed to correspond to the parameter value θ_0. This parameter often results from a preliminary identification based on reference data, as in module 3.2 .

Given a new N-size sample of sensors data, the following question is addressed : *Does the new sample still correspond to the nominal model* $\mathbf{P}_{\theta_0}$ *?* One manner to address this generally difficult question is the following. The asymptotic local approach consists in deciding between the nominal hypothesis and a *close* alternative hypothesis, namely :

$$\text{(Safe) } \mathbf{H}_0 : \ \theta = \theta_0 \quad \text{and} \quad \text{(Damaged) } \mathbf{H}_1 : \ \theta = \theta_0 + \eta/\sqrt{N} \tag{21}$$

where η is an unknown but fixed change vector. A residual is generated under the form :

$$\zeta_N = 1/\sqrt{N} \sum_{k=0}^{N} K(\theta_0, Z_k) = \sqrt{N}\, \mathcal{K}_N(\theta_0) \ . \tag{22}$$

If the matrix $\mathcal{J}_N = -\,\mathbf{E}_{\theta_0}[\partial \mathcal{K}_N(\theta_0)]$ converges towards a limit $\mathcal{J}$, then, under mild mixing and stationarity assumptions, the central limit theorem shows [60] that the residual is asymptotically Gaussian :

$$\zeta_N \xrightarrow[N \to \infty]{} \begin{cases} \mathcal{N}(0, \Sigma) & \text{under } \mathbf{P}_{\theta_0} \ , \\ \\ \mathcal{N}(\mathcal{J}\,\eta, \Sigma) & \text{under } \mathbf{P}_{\theta_0+\eta/\sqrt{N}} \ , \end{cases} \tag{23}$$

where the asymptotic covariance matrix Σ can be estimated, and manifests the deviation in the parameter vector by a change in its own mean value. Then, deciding between $\eta = 0$ and $\eta \neq 0$ amounts to compute the following χ^2-test, provided that $\mathcal{J}$ is full rank and Σ is invertible :

$$\chi^2 = \overline{\zeta}^T\, \mathbf{F}^{-1}\, \overline{\zeta} \gtrless \lambda \ . \tag{24}$$

where

$$\overline{\zeta} \triangleq \mathcal{J}^T \, \Sigma^{-1} \, \zeta_N \quad \text{and} \quad \mathbf{F} \triangleq \mathcal{J}^T \, \Sigma^{-1} \, \mathcal{J} \tag{25}$$

With this approach, it is possible to decide, with a quantifiable error level, if a residual value is significantly different from zero, for assessing whether a fault/damage has occurred. It should be stressed that the residual and the sensitivity and covariance matrices $\mathcal{J}$ and Σ can be evaluated (or estimated) for the nominal model. In particular, it is *not* necessary to re-identify the model, and the sensitivity and covariance matrices can be pre-computed off-line.

3.4. Diagnostics

A further monitoring step, often called *fault isolation*, consists in determining which (subsets of) components of the parameter vector θ have been affected by the change. Solutions for that are now described. How this relates to diagnostics is addressed afterwards.

The question: *which (subsets of) components of θ have changed ?*, can be addressed using either nuisance parameters elimination methods or a multiple hypotheses testing approach [59].

In most SHM applications, a complex physical system, characterized by a generally non identifiable parameter vector Φ has to be monitored using a simple (black-box) model characterized by an identifiable parameter vector θ. A typical example is the vibration monitoring problem for which complex finite elements models are often available but not identifiable, whereas the small number of existing sensors calls for identifying only simplified input-output (black-box) representations. In such a situation, two different diagnosis problems may arise, namely diagnosis in terms of the black-box parameter θ and diagnosis in terms of the parameter vector Φ of the underlying physical model.

The isolation methods sketched above are possible solutions to the former. Our approach to the latter diagnosis problem is basically a detection approach again, and not a (generally ill-posed) inverse problem estimation approach [3]. The basic idea is to note that the physical sensitivity matrix writes $\mathcal{J} \, \mathcal{J}_{\Phi\theta}$, where $\mathcal{J}_{\Phi\theta}$ is the Jacobian matrix at Φ_0 of the application $\Phi \mapsto \theta(\Phi)$, and to use the sensitivity test for the components of the parameter vector Φ. Typically this results in the following type of directional test :

$$\chi^2_\Phi = \zeta^T \, \Sigma^{-1} \, \mathcal{J} \, \mathcal{J}_{\Phi\theta} \, (\mathcal{J}^T_{\Phi\theta} \, \mathcal{J}^T \, \Sigma^{-1} \, \mathcal{J} \, \mathcal{J}_{\Phi\theta})^{-1} \, \mathcal{J}^T_{\Phi\theta} \, \mathcal{J}^T \, \Sigma^{-1} \, \zeta \gtrless \lambda \; . \tag{26}$$

It should be clear that the selection of a particular parameterization Φ for the physical model may have a non negligible influence on such type of tests, according to the numerical conditioning of the Jacobian matrices $\mathcal{J}_{\Phi\theta}$.

As a summary, the machinery in modules 3.2 , 3.3 and 3.4 provides us with a generic framework for designing monitoring algorithms for continuous structures, machines and processes. This approach assumes that a model of the monitored system is available. This is a reasonable assumption within the field of applications since most mechanical processes rely on physical principles which write in terms of equations, providing us with models. These important *modeling* and *parameterization* issues are among the questions we intend to investigate within our research program.

The key issue to be addressed within each parametric model class is the residual generation, or equivalently the choice of the *parameter estimating function*.

3.5. Subspace-based identification and detection

For reasons closely related to the vibrations monitoring applications, we have been investigating subspace-based methods, for both the identification and the monitoring of the eigenstructure (λ, ϕ_λ) of the state transition matrix F of a linear dynamical state-space system :

$$\left\{ \begin{array}{rcl} X_{k+1} & = & F\ X_k + V_{k+1} \\ Y_k & = & H\ X_k \end{array} \right. , \tag{27}$$

namely the $(\lambda, \varphi_\lambda)$ defined by :

$$\det\ (F - \lambda\ I) = 0, \quad (F - \lambda\ I)\ \phi_\lambda = 0, \quad \varphi_\lambda \triangleq H\ \phi_\lambda \tag{28}$$

The (canonical) parameter vector in that case is :

$$\theta \triangleq \begin{pmatrix} \Lambda \\ \mathrm{vec}\Phi \end{pmatrix} \tag{29}$$

where Λ is the vector whose elements are the eigenvalues λ, Φ is the matrix whose columns are the φ_λ's, and vec is the column stacking operator.

Subspace-based methods is the generic name for linear systems identification algorithms based on either time domain measurements or output covariance matrices, in which different subspaces of Gaussian random vectors play a key role [62]. A contribution of ours, minor but extremely fruitful, has been to write the output-only covariance-driven subspace identification method under a form that involves a parameter estimating function, from which we define a *residual adapted to vibration monitoring* [1]. This is explained next.

3.5.1. Covariance-driven subspace identification.

Let $R_i \triangleq \mathbf{E}\left(Y_k\ Y_{k-i}^T\right)$ and:

$$\mathcal{H}_{p+1,q} \triangleq \begin{pmatrix} R_0 & R_1 & \vdots & R_{q-1} \\ R_1 & R_2 & \vdots & R_q \\ \vdots & \vdots & \vdots & \vdots \\ R_p & R_{p+1} & \vdots & R_{p+q-1} \end{pmatrix} \triangleq \mathrm{Hank}\left(R_i\right) \tag{30}$$

be the output covariance and Hankel matrices, respectively; and: $G \triangleq \mathbf{E}\left(X_k Y_k^T\right)$. Direct computations of the R_i's from the equations (10) lead to the well known key factorizations :

$$\begin{array}{rcl} R_i & = & HF^iG \\ \mathcal{H}_{p+1,q} & = & \mathcal{O}_{p+1}(H,F)\ \mathcal{C}_q(F,G) \end{array} \tag{31}$$

where:

$$\mathcal{O}_{p+1}(H,F) \triangleq \begin{pmatrix} H \\ HF \\ \vdots \\ HF^p \end{pmatrix} \quad \text{and} \quad \mathcal{C}_q(F,G) \triangleq (G\ FG\ \cdots\ F^{q-1}G) \tag{32}$$

are the observability and controllability matrices, respectively. The observation matrix H is then found in the first block-row of the observability matrix $\mathcal{O}$. The state-transition matrix F is obtained from the shift invariance property of $\mathcal{O}$. The eigenstructure (λ, ϕ_λ) then results from (11).

Since the actual model order is generally not known, this procedure is run with increasing model orders.

3.5.2. Model parameter characterization.

Choosing the eigenvectors of matrix F as a basis for the state space of model (10) yields the following representation of the observability matrix:

$$\mathcal{O}_{p+1}(\theta) = \begin{pmatrix} \Phi \\ \Phi\Delta \\ \vdots \\ \Phi\Delta^p \end{pmatrix} \tag{33}$$

where $\Delta \triangleq \text{diag}(\Lambda)$, and Λ and Φ are as in (12). Whether a nominal parameter θ_0 fits a given output covariance sequence $(R_j)_j$ is characterized by [1]:

$$\mathcal{O}_{p+1}(\theta_0) \text{ and } \mathcal{H}_{p+1,q} \text{ have the same left kernel space.} \tag{34}$$

This property can be checked as follows. From the nominal θ_0, compute $\mathcal{O}_{p+1}(\theta_0)$ using (16), and perform e.g. a singular value decomposition (SVD) of $\mathcal{O}_{p+1}(\theta_0)$ for extracting a matrix U such that:

$$U^T\, U = I_s \text{ and } U^T\, \mathcal{O}_{p+1}(\theta_0) = 0 \tag{35}$$

Matrix U is not unique (two such matrices relate through a post-multiplication with an orthonormal matrix), but can be regarded as a function of θ_0. Then the characterization writes:

$$U(\theta_0)^T\, \mathcal{H}_{p+1,q} = 0 \tag{36}$$

3.5.3. Residual associated with subspace identification.

Assume now that *a reference* θ_0 *and a new sample* $Y_1, \cdots, Y_N$ *are available.* For checking whether the data agree with θ_0, the idea is to compute the empirical Hankel matrix $\widehat{\mathcal{H}}_{p+1,q}$:

$$\widehat{\mathcal{H}}_{p+1,q} \triangleq \text{Hank}\left(\widehat{R}_i\right), \quad \widehat{R}_i \triangleq 1/(N-i) \sum_{k=i+1}^{N} Y_k\, Y_{k-i}^T \tag{37}$$

and to define the residual vector:

$$\zeta_N(\theta_0) \triangleq \sqrt{N} \text{ vec}\left(U(\theta_0)^T\, \widehat{\mathcal{H}}_{p+1,q}\right) \tag{38}$$

Let θ be the actual parameter value for the system which generated the new data sample, and $\mathbf{E}_\theta$ be the expectation when the actual system parameter is θ. From (19), we know that $\zeta_N(\theta_0)$ has zero mean when no change occurs in θ, and nonzero mean if a change occurs. Thus $\zeta_N(\theta_0)$ plays the role of a residual.

It is our experience that this residual has highly interesting properties, both for damage detection [1] and localization [3], and for flutter monitoring [8].

3.5.4. Other uses of the key factorizations.

Factorization (3.5.1) is the key for a characterization of the canonical parameter vector θ in (12), and for deriving the residual. Factorization (14) is also the key for :

- Proving consistency and robustness results [6];
- Designing an extension of covariance-driven subspace identification algorithm adapted to the presence and fusion of non-simultaneously recorded multiple sensors setups [7];
- Proving the consistency and robustness of this extension [9];
- Designing various forms of *input-output* covariance-driven subspace identification algorithms adapted to the presence of both known inputs and unknown excitations [10].

3.5.5. Research program

The research will first focus on the extension and implementation of current techniques as developed in I4S and IFSTTAR. Before doing any temperature rejection on large scale structures as planned, we need to develop good and accurate models of thermal fields. We also need to develop robust and efficient versions of our algorithms, mainly the subspace algorithms before envisioning linking them with physical models. Briefly, we need to mature our statistical toolset as well as our physical modeling before mixing them together later on.

3.5.5.1. Direct vibration modeling under temperature changes

This task builds upon what has been achieved in the CONSTRUCTIF project, where a simple formulation of the temperature effect has been exhibited, based on relatively simple assumptions. The next step is to generalize this modeling to a realistic large structure under complex thermal changes. Practically, temperature and resulting structural prestress and pre strains of thermal origin are not uniform and civil structures are complex. This leads to a fully 3D temperature field, not just a single value. Inertia effects also forbid a trivial prediction of the temperature based on current sensor outputs while ignoring past data. On the other side, the temperature is seen as a nuisance. That implies that any damage detection procedure has first to correct the temperature effect prior to any detection.

Modeling vibrations of structures under thermal prestress does and will play an important role in the static correction of kinematic measurements, in health monitoring methods based on vibration analysis as well as in durability and in the active or semi-active control of civil structures that by nature are operated under changing environmental conditions. As a matter of fact, using temperature and dynamic models the project aims at correcting the current vibration state from induced temperature effects, such that damage detection algorithms rely on a comparison of this thermally corrected current vibration state with a reference state computed or measured at a reference temperature. This approach is expected to cure damage detection algorithms from the environmental variations.

I4S will explore various ways of implementing this concept, notably within the FUI SIPRIS project.

3.5.5.2. Damage localization algorithms (in the case of localized damages such as cracks)

During the CONSTRUCTIF project, both feasibility and efficiency of some damage detection and localization algorithms were proved. Those methods are based on the tight coupling of statistical algorithms with finite element models. It has been shown that effective localization of some damaged elements was possible, and this was validated on a numerical simulated bridge deck model. Still, this approach has to be validated on real structures.

On the other side, new localization algorithms are currently investigated such as the one developed conjointly with University of Boston and tested within the framework of FP7 ISMS project. These algorithms will be implemented and tested on the PEGASE platform as well as all our toolset.

When possible, link with temperature rejection will be done along the lines of what has been achieved in the CONSTRUCTIF project.

3.5.5.3. Uncertainty quantification for system identification algorithms

Some emphasis will be put on expressing confidence intervals for system identification. It is a primary goal to take into account the uncertainty within the identification procedure, using either identification algorithms derivations or damage detection principles. Such algorithms are critical for both civil and aeronautical structures monitoring. It has been shown that confidence intervals for estimation parameters can theoretically be related to the damage detection techniques and should be computed as a function of the Fisher information matrix associated to the damage detection test. Based on those assumptions, it should be possible to obtain confidence intervals for a large class of estimates, from damping to finite elements models. Uncertainty considerations are also deeply investigated in collaboration with Dassault Aviation in Mellinger PhD thesis or with Northeastern University, Boston, within Gallegos PhD thesis.

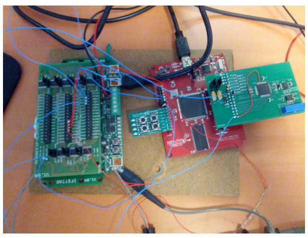
3.5.5.4. Reflectometry-based methods for civil engineering structure health monitoring

For mechanical structures with a dominating geometrical axis so that they can be approximately considered one dimensional structures, some reflectometry-based methods initially developed for electrical cable monitoring have proved efficient for their health monitoring. Typical applications of such methods have been validated for the monitoring of external post-tensioned cables built with concrete bridges. Further studies are necessary to generalize this technology to other mechanical structures.

3.5.5.5. PEGASE platform

A new iteration called PEGASE 2 of our wireless platform has to be finalized (see Software section), in particular:

- Validation of PEGASE 2 mother board for its ability to recover energy from solar cells. Writing resulting abacus and user-guides...
- Discover and manage the DSP Library of PEGASE 2 (TI 5330 processor)
- Finalizing its main daughter boards:
  - 8 synchronous analog channel daughter board (finalized at 90
  - validation of the POE (Power Over Ethernet) daughter board
  - validation of the 3G daughter board (for GSM links)
  - Finalizing the supervisor (Matlab plugin...)



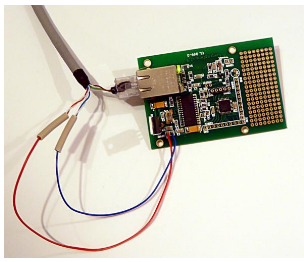


Figure 1. PEGASE board

Maxplus Project-Team

3. Research Program

3.1. L'algèbre max-plus/Max-plus algebra

Le semi-corps *max-plus* est l'ensemble $\mathbb{R} \cup \{-\infty\}$, muni de l'addition $(a, b) \mapsto a \oplus b = \max(a, b)$ et de la multiplication $(a, b) \mapsto a \otimes b = a + b$. Cette structure algébrique diffère des structures de corps classiques par le fait que l'addition n'est pas une loi de groupe, mais est idempotente: $a \oplus a = a$. On rencontre parfois des variantes de cette structure: par exemple, le semi-corps *min-plus* est l'ensemble $\mathbb{R} \cup \{+\infty\}$ muni des lois $a \oplus b = \min(a, b)$ et $a \otimes b = a + b$, et le semi-anneau *tropical* est l'ensemble $\mathbb{N} \cup \{+\infty\}$ munis des mêmes lois. L'on peut se poser la question de généraliser les constructions de l'algèbre et de l'analyse classique, qui reposent pour une bonne part sur des anneaux ou des corps tels que $\mathbb{Z}$ ou $\mathbb{R}$, au cas de semi-anneaux de type max-plus: tel est l'objet de ce qu'on appelle un peu familièrement "l'algèbre max-plus".

Il est impossible ici de donner une vue complète du domaine. Nous nous bornerons à indiquer quelques références bibliographiques. L'intérêt pour les structures de type max-plus est contemporain de la naissance de la théorie des treillis [114]. Depuis, les structures de type max-plus ont été développées indépendamment par plusieurs écoles, en relation avec plusieurs domaines. Les motivations venant de la Recherche Opérationnelle (programmation dynamique, problèmes de plus court chemin, problèmes d'ordonnancement, optimisation discrète) ont été centrales dans le développement du domaine [103], [134], [183], [187], [188]. Les semi-anneaux de type max-plus sont bien sûr reliés aux algèbres de Boole [90]. L'algèbre max-plus apparaît de manière naturelle en contrôle optimal et dans la théorie des équations aux dérivées partielles d'Hamilton-Jacobi [173], [171], [157], [141], [130], [176], [150], [131], [117], [65]. Elle apparaît aussi en analyse asymptotique (asymptotiques de type WKB [156], [157], [141], grandes déviations [170], asymptotiques à température nulle en physique statistique [92]), puisque l'algèbre max-plus apparaît comme limite de l'algèbre usuelle. La théorie des opérateurs linéaires max-plus peut être vue comme faisant partie de la théorie des opérateurs de Perron-Frobenius non-linéaires, ou de la théorie des applications contractantes ou monotones sur les cônes [142], [161], [154], [79], laquelle a de nombreuse motivations, telles l'économie mathématique [159], et la théorie des jeux [174], [54]. Dans la communauté des systèmes à événements discrets, l'algèbre max-plus a été beaucoup étudiée parce qu'elle permet de représenter de manière linéaire les phénomènes de synchronisation, lesquels déterminent le comportement temporel de systèmes de production ou de réseaux, voir [6]. Parmi les développements récents du domaine, on peut citer le calcul des réseaux [91], [146], qui permet de calculer des bornes pire des cas de certaines mesures de qualité de service. En informatique théorique, l'algèbre max-plus (ou plutôt le semi-anneau tropical) a joué un rôle décisif dans la résolution de problèmes de décision en théorie des automates [178], [137], [179], [143], [163]. Notons finalement, pour information, que l'algèbre max-plus est apparue récemment en géométrie algébrique [129], [182], [158], [181] et en théorie des représentations [118], [82], sous les noms de géométrie et combinatoire tropicales.

Nous décrivons maintenant de manière plus détaillée les sujets qui relèvent directement des intérêts du projet, comme la commande optimale, les asymptotiques, et les systèmes à événements discrets.

English version

The *max-plus* semifield is the set $\mathbb{R} \cup \{-\infty\}$, equipped with the addition $(a, b) \mapsto a \oplus b = \max(a, b)$ and the multiplication $(a, b) \mapsto a \otimes b = a + b$. This algebraic structure differs from classical structures, like fields, in that addition is idempotent: $a \oplus a = a$. Several variants have appeared in the literature: for instance, the *min-plus* semifield is the set $\mathbb{R} \cup \{+\infty\}$ equipped with the laws $a \oplus b = \min(a, b)$ and $a \otimes b = a + b$, and the *tropical* semiring is the set $\mathbb{N} \cup \{+\infty\}$ equipped with the same laws. One can ask the question of extending to max-plus type structures the classical constructions and results of algebra and analysis: this is what is often called in a wide sense "max-plus algebra" or "tropical algebra".

It is impossible to give in this short space a fair view of the field. Let us, however, give a few references. The interest in max-plus type structures is contemporaneous with the early developments of lattice theory [114]. Since that time, max-plus structures have been developed independently by several schools, in relation with several fields. Motivations from Operations Research (dynamic programming, shortest path problems, scheduling problems, discrete optimisation) were central in the development of the field [103], [134], [183], [187], [188]. Of course, max-plus type semirings are related to Boolean algebras [90]. Max-plus algebras arises naturally in optimal control and in the theory of Hamilton-Jacobi partial differential equations [173], [171], [157], [141], [130], [176], [150], [131], [117], [65]. It arises in asymptotic analysis (WKB asymptotics [156], [157], [141], large deviation asymptotics [170], or zero temperature asymptotics in statistical physics [92]), since max-plus algebra appears as a limit of the usual algebra. The theory of max-plus linear operators may be thought of as a part of the non-linear Perron-Frobenius theory, or of the theory of nonexpansive or monotone operators on cones [142], [161], [154], [79], a theory with numerous motivations, including mathematical economy [159] and game theory [174], [54]. In the discrete event systems community, max-plus algebra has been much studied since it allows one to represent linearly the synchronisation phenomena which determine the time behaviour of manufacturing systems and networks, see [6]. Recent developments include the network calculus of [91], [146] which allows one to compute worst case bounds for certain measures of quality of service. In theoretical computer science, max-plus algebra (or rather, the tropical semiring) played a key role in the solution of decision problems in automata theory [178], [137], [179], [143], [163]. We finally note for information that max-plus algebra has recently arisen in algebraic geometry [129], [182], [158], [181] and in representation theory [118], [82], under the names of tropical geometry and combinatorics.

We now describe in more details some parts of the subject directly related to our interests, like optimal control, asymptotics, and discrete event systems.

3.2. Algèbre max-plus, programmation dynamique, et commande optimale/Max-plus algebra, dynamic programming, and optimal control

L'exemple le plus simple d'un problème conduisant à une équation min-plus linéaire est le problème classique du plus court chemin. Considérons un graphe dont les nœuds sont numérotés de 1 à n et dont le coût de l'arc allant du nœud i au nœud j est noté $M_{ij} \in \mathbb{R} \cup \{+\infty\}$. Le coût minimal d'un chemin de longueur k, allant de i à j, est donné par la quantité:

$$v_{ij}(k) = \min_{\ell:\ \ell_0=i,\ \ell_k=j} \sum_{r=0}^{k-1} M_{\ell_r \ell_{r+1}} \ , \tag{39}$$

où le minimum est pris sur tous les chemins $\ell = (\ell_0, ..., \ell_k)$ de longueur k, de nœud initial $\ell_0 = i$ et de nœud final $\ell_k = j$. L'équation classique de la programmation dynamique s'écrit:

$$v_{ij}(k) = \min_{1 \le s \le n} (M_{is} + v_{sj}(k-1)) \ . \tag{40}$$

On reconnaît ainsi une équation linéaire min-plus :

$$v(k) = Mv(k-1) \ , \tag{41}$$

où on note par la concaténation le produit matriciel induit par la structure de l'algèbre min-plus. Le classique *problème de Lagrange* du calcul des variations,

$$v(x,T) = \inf_{X(\cdot),\ X(0)=x} \int_0^T L(X(t), \dot{X}(t))\mathrm{d}t + \phi(X(T)) \ , \tag{42}$$

où $X(t) \in \mathbb{R}^n$, pour $0 \le t \le T$, et $L : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ est le Lagrangien, peut être vu comme une version continue de (1), ce qui permet de voir l'équation d'Hamilton-Jacobi que vérifie v,

$$v(\cdot,0)=\phi, \quad \frac{\partial v}{\partial T}+H(x,\frac{\partial v}{\partial x})=0, \qquad H(x,p)=\sup_{y\in\mathbb{R}^n}\left(-p\cdot y-L(x,y)\right) \ , \tag{43}$$

comme une équation min-plus linéaire. En particulier, les solutions de (5) vérifient un principe de superposition min-plus: si v et w sont deux solutions, et si $\lambda, \mu \in \mathbb{R}$, $\inf(\lambda+v, \mu+w)$ est encore solution de (5). Ce point de vue, inauguré par Maslov, a conduit au développement de l'école d'Analyse Idempotente (voir [157], [141], [150]).

La présence d'une structure algébrique sous-jacente permet de voir les solutions stationnaires de (2) et (5) comme des vecteurs propres de la matrice M ou du semi-groupe d'évolution de l'équation d'Hamilton-Jacobi. La valeur propre associée fournit le coût moyen par unité de temps (coût ergodique). La représentation des vecteurs propres (voir [173], [183], [103], [132], [97], [78], [6] pour la dimension finie, et [157], [141] pour la dimension infinie) est intimement liée au théorème de l'autoroute qui décrit les trajectoires optimales quand la durée ou la longueur des chemins tend vers l'infini. Pour l'équation d'Hamilton-Jacobi, des résultats reliés sont apparus récemment en théorie d'"Aubry-Mather" [117].

English version

The most elementary example of a problem leading to a min-plus linear equation is the classical shortest path problem. Consider a graph with nodes $1, ..., n$, and let $M_{ij} \in \mathbb{R} \cup \{+\infty\}$ denote the cost of the arc from node i to node j. The minimal cost of a path of a given length, k, from i to j, is given by (1), where the minimum is taken over all paths $\ell = (\ell_0, ..., \ell_k)$ of length k, with initial node $\ell_0 = i$ and final node $\ell_k = j$. The classical dynamic programming equation can be written as in (2). We recognise the min-plus linear equation (3), where concatenation denotes the matrix product induced by the min-plus algebraic structure. The classical *Lagrange problem* of calculus of variations, given by (4) where $X(t) \in \mathbb{R}^n$, for $0 \le t \le T$, and $L : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is the Lagrangian, may be thought of as a continuous version of (1), which allows us to see the Hamilton-Jacobi equation (5) satisfied by v, as a min-plus linear equation. In particular, the solutions of (5) satisfy a min-plus superposition principle: if v and w are two solutions, and if $\lambda, \mu \in \mathbb{R}$, then $\inf(\lambda+v, \mu+w)$ is also a solution of (5). This point of view, due to Maslov, led to the developpement of the school of Idempotent Analysis (see [157], [141], [150]).

The underlying algebraic structure allows one to see stationnary solutions of (2) and (5) as eigenvectors of the matrix M or of the evolution semigroup of the Hamilton-Jacobi equation. The associated eigenvalue gives the average cost per time unit (ergodic cost). The representation of eigenvectors (see [173], [183], [132], [97], [103], [78], [6] for the finite dimension case, and [157], [141] for the infinite dimension case) is intimately related to turnpike theorems, which describe optimal trajectories as the horizon, or path length, tends to infinity. For the Hamilton-Jacobi equation, related results have appeared recently in the "Aubry-Mather" theory [117].

3.3. Applications monotones et théorie de Perron-Frobenius non-linéaire, ou l'approche opératorielle du contrôle optimal et des jeux/Monotone maps and non-linear Perron-Frobenius theory, or the operator approach to optimal control and games

On sait depuis le tout début des travaux en décision markovienne que les opérateurs de la programmation dynamique f de problèmes de contrôle optimal ou de jeux (à somme nulle et deux joueurs), avec critère additif, ont les propriétés suivantes :

$$\begin{array}{llcl} \text{monotonie}/\textit{monotonicity} & x \le y & \Rightarrow & f(x) \le f(y) \ , \\ \text{contraction}/\textit{nonexpansiveness} & \|f(x)-f(y)\|_\infty & \le & \|x-y\|_\infty \ . \end{array} \tag{44}$$

Ici, l'opérateur f est une application d'un certain espace de fonctions à valeurs réelles dans lui-même, $\leq$ désigne l'ordre partiel usuel, et $\|\cdot\|_\infty$ désigne la norme sup. Dans le cas le plus simple, l'ensemble des états est $\{1,...,n\}$ et f est une application de $\mathbb{R}^n$ dans lui-même. Les applications monotones qui sont contractantes pour la norme du sup peuvent être vues comme des généralisations non-linéaires des matrices sous-stochastiques. Une sous-classe utile, généralisant les matrices stochastiques, est formée des applications qui sont monotones et commutent avec l'addition d'une constante [102] (celles ci sont parfois appelées fonctions topicales). Les problèmes de programmation dynamique peuvent être traduits en termes d'opérateurs : l'équation de la programmation dynamique d'un problème de commande optimale à horizon fini s'écrit en effet $x(k) = f(x(k-1))$, où $x(k)$ est la fonction valeur en horizon k et $x(0)$ est donné; la fonction valeur y d'un problème à horizon infini (y compris le cas d'un problème d'arrêt optimal) vérifie $y = f(y)$; la fonction valeur z d'un problème avec facteur d'actualisation $0 < \alpha < 1$ vérifie $z = f(\alpha z)$, etc. Ce point de vue abstrait a été très fructueux, voir par exemple [54]. Il permet d'inclure la programmation dynamique dans la perspective plus large de la théorie de Perron-Frobenius non-linéaire, qui, depuis l'extension du théorème de Perron-Frobenius par Krein et Rutman, traite des applications non linéaires sur des cônes vérifiant des conditions de monotonie, de contraction ou d'homogénéité. Les problèmes auxquels on s'intéresse typiquement sont la structure de l'ensemble des points fixes de f, le comportement asymptotique de f^k, en particulier l'existence de la limite de $f^k(x)/k$ lorsque k tends vers l'infini (afin d'obtenir le coût ergodique d'un problème de contrôle optimal ou de jeux), l'asymptotique plus précise de f^k, à une normalisation près (afin d'obtenir le comportement précis de l'itération sur les valeurs), etc. Nous renvoyons le lecteur à [161] pour un panorama. Signalons que dans [123],[7], des algorithmes inspirés de l'algorithme classique d'itérations sur les politiques du contrôle stochastique ont pu être introduits dans le cas des opérateurs monotones contractants généraux, en utilisant des résultats de structure de l'ensemble des points fixes de ces opérateurs. Les applications de la théorie des applications monotones contractantes ne se limitent pas au contrôle optimal et aux jeux. En particulier, on utilise la même classe d'applications dans la modélisation des systèmes à événements discrets, voir le §3.5 ci-dessous, et une classe semblable d'applications en analyse statique de programmes, voir §4.4 ci-dessous.

English version

Since the very beginning of Markov decision theory, it has been observed that dynamic programming operators f arising in optimal control or (zero-sum, two player) game problems have Properties (6). Here, the operator f is a self-map of a certain space of real valued functions, equipped with the standard ordering $\leq$ and with the sup-norm $\|\cdot\|_\infty$. In the simplest case, the set of states is $\{1,...,n\}$, and f is a self-map of $\mathbb{R}^n$. Monotone maps that are nonexpansive in the sup norm may be thought of as nonlinear generalisations of substochastic matrices. A useful subclass, which generalises stochastic matrices, consists of those maps which are monotone and commute with the addition of a constant [102] (these maps are sometimes called topical functions). Dynamic programming problems can be translated in operator terms: the dynamic programming equation for a finite horizon problem can be written as $x(k) = f(x(k-1))$, where $x(k)$ is the value function in horizon k and $x(0)$ is given; the value function y of a problem with an infinite horizon (including the case of optimal stopping) satisfies $y = f(y)$; the value function z of a problem with discount factor $0 < \alpha < 1$ satisfies $z = f(\alpha z)$, etc. This abstract point of view has been very fruitful, see for instance [54]. It allows one to put dynamic programming in the wider perspective of nonlinear Perron-Frobenius theory, which, after the extension of the Perron-Frobenius theorem by Krein and Rutman, studies non-linear self-maps of cones, satisfying various monotonicity, nonexpansiveness, and homogeneity conditions. Typical problems of interests are the structure of the fixed point set of f, the asymptotic behaviour of f^k, including the existence of the limit of $f^k(x)/k$ as k tends to infinity (which yields the ergodic cost in control or games problems), the finer asymptotic behaviour of f^k, possibly up to a normalisation (which yields precise results on value iteration), etc. We shall not attempt to survey this theory here, and will only refer the reader to [161] for more background. In [123],[7], algorithms inspired from the classical policy iterations algorithm of stochastic control have been introduced for general monotone nonexpansive operators, using structural results for the fixed point set of these operators. Applications of monotone or nonexpansive maps are not limited to optimal control and game theory. In particular, we also use the same class of maps as models of discrete event dynamics systems, see §3.5 below, and we shall see in §4.4 that related classes of maps are useful in the static analysis of computer programs.

3.4. Processus de Bellman/Bellman processes

Un autre point de vue sur la commande optimale est la théorie des *processus de Bellman* [171], [107], [106], [65],[1], qui fournit un analogue max-plus de la théorie des probabilités. Cette théorie a été développée à partir de la notion de *mesure idempotente* introduite par Maslov [156]. Elle établit une correspondance entre probabilités et optimisation, dans laquelle les variables aléatoires deviennent des variables de coût (qui permettent de paramétriser les problèmes d'optimisation), la notion d'espérance conditionnelle est remplacée par celle de coût conditionnel (pris sur un ensemble de solutions faisables), la propriété de Markov correspond au principe de la programmation dynamique de Bellman, et la convergence faible à une convergence de type épigraphe. Les théorèmes limites pour les processus de Bellman (loi des grands nombres, théorème de la limite centrale, lois stables) fournissent des résultats asymptotiques en commande optimale. Ces résultats généraux permettent en particulier de comprendre qualitativement les difficultés d'approximation des solutions d'équations d'Hamilton-Jacobi retrouvés en particulier dans le travail de thèse d'Asma Lakhoua [144], [62].

English version

Another point of view on optimal control is the theory of *Bellman processes* [171], [107], [106], [65], [1] which provides a max-plus analogue of probability theory, relying on the theory of *idempotent measures* due to Maslov [156]. This establishes a correspondence between probability and optimisation, in which random variables become cost variables (which allow to parametrise optimisation problems), the notion of conditional expectation is replaced by a notion of conditional cost (taken over a subset of feasible solutions), the Markov property corresponds to the Bellman's dynamic programming principle, and weak convergence corresponds to an epigraph-type convergence. Limit theorems for Bellman processes (law of large numbers, central limit theorems, stable laws) yield asymptotic results in optimal control. Such general results help in particular to understand qualitatively the difficulty of approximation of Hamilton-Jacobi equations found again in particular in the PhD thesis work of Asma Lakhoua [144], [62].

3.5. Systèmes à événements discrets/Discrete event systems

Des systèmes dynamiques max-plus linéaires, de type (2), interviennent aussi, avec une interprétation toute différente, dans la modélisation des systèmes à événements discrets. Dans ce contexte, on associe à chaque tâche répétitive, i, une fonction *compteur*, $v_i : \mathbb{R} \to \mathbb{N}$, telle que $v_i(t)$ compte le nombre cumulé d'occurrences de la tâche i jusqu'à l'instant t. Par exemple, dans un système de production, $v_i(t)$ compte le nombre de pièces d'un certain type produites jusqu'à l'instant t. Dans le cas le plus simple, qui dans le langage des réseaux de Petri, correspond à la sous-classe très étudiée des graphes d'événements temporisés [93], on obtient des équations min-plus linéaires analogues à (2). Cette observation, ou plutôt, l'observation duale faisant intervenir des fonctions dateurs, a été le point de départ [97] de l'approche max-plus des systèmes à événements discrets [6], qui fournit un analogue max-plus de la théorie des systèmes linéaires classiques, incluant les notions de représentation d'état, de stabilité, de séries de transfert, etc. En particulier, les valeurs propres fournissent des mesures de performance telles que le taux de production. Des généralisations non-linéaires, telles que les systèmes dynamiques min-max [162], [136], ont aussi été étudiées. Les systèmes dynamiques max-plus linéaires aléatoires sont particulièrement utiles dans la modélisation des réseaux [77]. Les modèles d'automates à multiplicités max-plus [121], incluant certains versions temporisées des modèles de traces ou de tas de pièces [125], permettent de représenter des phénomènes de concurrence ou de partage de ressources. Les automates à multiplicités max-plus on été très étudiés par ailleurs en informatique théorique [178], [137], [149], [179], [143], [163]. Ils fournissent des modèles particulièrement adaptés à l'analyse de problèmes d'ordonnancement [148].

English version

Dynamical systems of type (2) also arise, with a different interpretation, in the modelling of discrete event systems. In this context, one associates to every repetitive task, i, a counter function, $v_i : \mathbb{R} \to \mathbb{N}$, such that $v_i(t)$ gives the total number of occurrences of task i up to time t. For instance, in a manufacturing system, $v_i(t)$ will count the number of parts of a given type produced up to time t. In the simplest case, which, in the vocabulary of Petri nets, corresponds to the much studied subclass of timed event graphs [93], we get min-plus linear equations similar to (2). This observation, or rather, the dual observation concerning dater functions, was the starting point [97] of the max-plus approach of discrete event systems [6], which provides some analogue of the classical linear control theory, including notions of state space representations, stability, transfer series, etc. In particular, eigenvalues yield performance measures like the throughput. Nonlinear generalisations, like min-max dynamical systems [162], [136], have been particularly studied. Random max-plus linear dynamical systems are particularly useful in the modelling of networks [77]. Max-plus automata models [121], which include some timed version of trace or heaps of pieces models [125], allow to represent phenomena of concurrency or resource sharing. Note that max-plus automata have been much studied in theoretical computer science [178], [137], [149], [179], [143], [163]. Such automata models are particularly adapted to the analysis of scheduling problems [148].

3.6. Algèbre linéaire max-plus/Basic max-plus algebra

Une bonne partie des résultats de l'algèbre max-plus concerne l'étude des systèmes d'équations linéaires. On peut distinguer trois familles d'équations, qui sont traitées par des techniques différentes : 1) Nous avons déjà évoqué dans les sections 3.2 et 3.3 le problème spectral max-plus $Ax = \lambda x$ et ses généralisations. Celui-ci apparaît en contrôle optimal déterministe et dans l'analyse des systèmes à événements discrets. 2) Le problème $Ax = b$ intervient en commande juste-à-temps (dans ce contexte, le vecteur x représente les dates de démarrage des tâches initiales, b représente certaines dates limites, et on se contente souvent de l'inégalité $Ax \leq b$). Le problème $Ax = b$ est intimement lié au problème d'affectation optimale, et plus généralement au problème de transport optimal. Il se traite via la théorie des correspondances de Galois abstraites, ou théorie de la résiduation [114], [84], [183], [187],[6]. Les versions dimension infinie du problème $Ax = b$ sont reliées aux questions d'analyse convexe abstraite [180], [175], [60] et de dualité non convexe. 3) Le problème linéaire général $Ax = Bx$ conduit à des développements combinatoires intéressants (polyèdres max-plus, déterminants max-plus, symétrisation [135], [164],[6]). Le sujet fait l'objet d'un intérêt récemment renouvelé [108].

English version

An important class of results in max-plus algebra concerns the study of max-plus linear equations. One can distinguish three families of equations, which are handled using different techniques: 1) We already mentioned in Sections 3.2 and 3.3 the max-plus spectral problem $Ax = \lambda x$ and its generalisations, which appears in deterministic optimal control and in performance analysis of discrete event systems. 2) The $Ax = b$ problem arises naturally in just in time problems (in this context, the vector x represents the starting times of initial tasks, b represents some deadlines, and one is often content with the inequality $Ax \leq b$). The $Ax = b$ problem is intimately related with optimal assignment, and more generally, with optimal transportation problems. Its theory relies on abstract Galois correspondences, or residuation theory [114], [84], [183], [187],[6]. Infinite dimensional versions of the $Ax = b$ problem are related to questions of abstract convex analysis [180], [175], [60] and nonconvex duality. 3) The general linear system $Ax = Bx$ leads to interesting combinatorial developments (max-plus polyhedra, determinants, symmetrisation [135], [164],[6]). The subject has attracted recently a new attention [108].

3.7. Algèbre max-plus et asymptotiques/Using max-plus algebra in asymptotic analysis

Le rôle de l'algèbre min-plus ou max-plus dans les problèmes asymptotiques est évident si l'on écrit

$$e^{-a/\epsilon} + e^{-b/\epsilon} \asymp e^{-\min(a,b)/\epsilon} \quad , \qquad e^{-a/\epsilon} \times e^{-b/\epsilon} = e^{-(a+b)/\epsilon} \quad , \tag{45}$$

lorsque $\epsilon \to 0^+$. Formellement, l'algèbre min-plus peut être vue comme la limite d'une déformation de l'algèbre classique, en introduisant le semi-anneau $\mathbb{R}_\epsilon$, qui est l'ensemble $\mathbb{R} \cup \{+\infty\}$, muni de l'addition $(a, b) \mapsto -\epsilon \log (e^{-a/\epsilon} + e^{-b/\epsilon})$ et de la multiplication $(a, b) \mapsto a + b$. Pour tout $\epsilon > 0$, $\mathbb{R}_\epsilon$ est isomorphe au semi-corps usuel des réels positifs, $(\mathbb{R}_+, +, \times)$, mais pour $\epsilon = 0^+$, $\mathbb{R}_\epsilon$ n'est autre que le semi-anneau min-plus. Cette idée a été introduite par Maslov [156], motivé par l'étude des asymptotiques de type WKB d'équations de Schrödinger. Ce point de vue permet d'utiliser des résultats algébriques pour résoudre des problèmes d'asymptotiques, puisque les équations limites ont souvent un caractère min-plus linéaire.

Cette déformation apparaît classiquement en théorie des grandes déviations à la loi des grands nombres : dans ce contexte, les objets limites sont des mesures idempotentes au sens de Maslov. Voir [1], [170], [61], pour les relations entre l'algèbre max-plus et les grandes déviations, voir aussi [57], [56], [55] pour des applications de ces idées aux perturbations singulières de valeurs propres. La même déformation est à l'origine de nombreux travaux actuels en géométrie tropicale, à la suite de Viro [182].

English version

The role of min-plus algebra in asymptotic problems becomes obvious when writing Equations (7) when $\epsilon \to 0^+$. Formally, min-plus algebra may be thought of as the limit of a deformation of classical algebra, by introducing the semi-field $\mathbb{R}_\epsilon$, which is the set $\mathbb{R} \cup \{+\infty\}$, equipped with the addition $(a, b) \mapsto -\epsilon \log (e^{-a/\epsilon} + e^{-b/\epsilon})$ and the multiplication $(a, b) \mapsto a + b$. For all $\epsilon > 0$, $\mathbb{R}_\epsilon$ is isomorphic to the semi-field of usual real positive numbers, $(\mathbb{R}_+, +, \times)$, but for $\epsilon = 0^+$, $\mathbb{R}_\epsilon$ coincides with the min-plus semiring. This idea was introduced by Maslov [156], motivated by the study of WKB-type asymptotics of Schrödinger equations. This point of view allows one to use algebraic results in asymptotics problems, since the limit equations have often some kind of min-plus linear structure.

This deformation appears classically in large deviation theory: in this context, the limiting objects are idempotent measures, in the sense of Maslov. See [1], [170], [61] for the relation between max-plus algebra and large deviations. See also [57], [56], [55] for the application of such ideas to singular perturbation problems for matrix eigenvalues. The same deformation is at the origin of many current works in tropical geometry, in the line initiated by Viro [182].

MCTAO Project-Team

3. Research Program

3.1. Control Systems

Our effort is directed toward efficient methods for the *control* of real (physical) systems, based on a *model* of the system to be controlled. *System* refers to the physical plant or device, whereas *model* refers to a mathematical representation of it.

We mostly investigate nonlinear systems whose nonlinearities admit a strong structure derived from physics; the equations governing their behavior are then well known, and the modeling part consists in choosing what phenomena are to be retained in the model used for control design, the other phenomena being treated as perturbations; a more complete model may be used for simulations, for instance. We focus on systems that admit a reliable finite-dimensional model, in continuous time; this means that models are controlled ordinary differential equations, often nonlinear.

Choosing accurate models yet simple enough to allow control design is in itself a key issue; however, modeling or identification as a theory is not per se in the scope of our project.

The extreme generality and versatility of linear control do not contradict the often heard sentence "most real life systems are nonlinear". Indeed, for many control problems, a linear model is sufficient to capture the important features for control. The reason is that most control objectives are local, first order variations around an operating point or a trajectory are governed by a linear control model, and except in degenerate situations (non-controllability of this linear model), the local behavior of a nonlinear dynamic phenomenon is dictated by the behavior of first order variations. Linear control is the hard core of control theory and practice; it has been pushed to a high degree of achievement –see for instance some classics: [45], [35]– that leads to big successes in industrial applications (PID, Kalman filtering, frequency domain design, H^∞ robust control, etc...). It must be taught to future engineers, and it is still a topic of ongoing research.

Linear control by itself however reaches its limits in some important situations:

1. **Non local control objectives.** For instance, steering the system from a region to a reasonably remote other one (path planning and optimal control); in this case, local linear approximation cannot be sufficient.
   It is also the case when some domain of validity (e.g. stability) is prescribed and is larger than the region where the linear approximation is dominant.
2. **Local control at degenerate equilibria.** Linear control yields local stabilization of an equilibrium point based on the tangent linear approximation if the latter is controllable. When it is *not*, and this occurs in some physical systems at interesting operating points, linear control is irrelevant and specific nonlinear techniques have to be designed.
   This is in a sense an extreme case of the second paragraph in point 1 : the region where the linear approximation is dominant vanishes.
3. **Small controls.** In some situations, actuators only allow a very small magnitude of the effect of control compared to the effect of other phenomena. Then the behavior of the system without control plays a major role and we are again outside the scope of linear control methods.
4. **Local control around a trajectory.** Sometimes a trajectory has been selected (this appeals to point 1), and local regulation around this reference is to be performed. Linearization in general yields, when the trajectory is not a single equilibrium point, a *time-varying* linear system. Even if it is controllable, time-varying linear systems are not in the scope of most classical linear control methods, and it is better to incorporate this local regulation in the nonlinear design, all the more so as the linear approximation along optimal trajectories is, by nature, often non controllable.

Let us discuss in more details some specific problems that we are studying or plan to study: classification and structure of control systems in section 3.2 , optimal control, and its links with feedback, in section 3.3 , the problem of optimal transport in section 3.4 , and finally problems relevent to a specific class of systems where the control is "small" in section 3.5 .

3.2. Structure of nonlinear control systems

In most problems, choosing the proper coordinates, or the right quantities that describe a phenomenon, sheds light on a path to the solution. In control systems, it is often crucial to analyze the structure of the model, deduced from physical principles, of the plant to be controlled; this may lead to putting it via some transformations in a simpler form, or a form that is most suitable for control design. For instance, equivalence to a linear system may allow to use linear control; also, the so-called "flatness" property drastically simplifies path planning [40], [51].

A better understanding of the "set of nonlinear models", partly classifying them, has another motivation than facilitating control design for a given system and its model: it may also be a necessary step towards a theory of "nonlinear identification" and modeling. Linear identification is a mature area of control science; its success is mostly due to a very fine knowledge of the structure of the class of linear models: similarly, any progress in the understanding of the structure of the class of nonlinear models would be a contribution to a possible theory of nonlinear identification.

These topics are central in control theory, but raise very difficult mathematical questions: static feedback classification is a geometric problem which is feasible in principle, although describing invariants explicitly is technically very difficult; and conditions for dynamic feedback equivalence and linearization raise unsolved mathematical problems, that make one wonder about decidability [0].

3.3. Optimal control and feedback control, stabilization

3.3.1. Optimal control.

Mathematically speaking, optimal control is the modern branch of the calculus of variations, rather well established and mature [18], [49], [26], [58]. Relying on Hamiltonian dynamics is now prevalent, instead of the standard Lagrangian formalism of the calculus of variations. Also, coming from control engineering, constraints on the control (for instance the control is a force or a torque, which are naturally bounded) or the state (for example in the shuttle atmospheric re-entry problem there is a constraint on the thermal flux) are imposed; the ones on the state are usual but these on the state yield more complicated necessary optimality conditions and an increased intrinsic complexity of the optimal solutions. Also, in the modern treatment, ad-hoc numerical schemes have to be derived for effective computations of the optimal solutions.

What makes optimal control an applied field is the necessity of computing these optimal trajectories, or rather the controls that produce these trajectories (or, of course, close-by trajectories). Computing a given optimal trajectory and its control as a function of time is a demanding task, with non trivial numerical difficulties: roughly speaking, the Pontryagin Maximum Principle gives candidate optimal trajectories as solutions of a two point boundary value problem (for an ODE) which can be analyzed using mathematical tools from geometric control theory or solved numerically using shooting methods. Obtaining the *optimal synthesis* –the optimal control as a function of the state– is of course a more intricate problem [26], [31].

[0]Consider the simple system with state $(x, y, z) \in I\!R^3$ and two controls that reads $\dot{z} = (\dot{y} - z\dot{x})^2\dot{x}$ after elimination of the controls; it is not known whether it is equivalent to a linear system, or flat; this is because the property amounts to existence of a formula giving the general solution as a function of two arbitrary functions of time and their derivatives up to a certain order, but no bound on this order is known a priori, even for this very particular example.

These questions are not only academic for minimizing a cost is *very* relevant in many control engineering problems. However, modern engineering textbooks in nonlinear control systems like the “best-seller” [42] hardly mention optimal control, and rather put the emphasis on designing a feedback control, as regular and explicit as possible, satisfying some qualitative (and extremely important!) objectives: disturbance attenuation, decoupling, output regulation or stabilization. Optimal control is sometimes viewed as disconnected from automatic control... we shall come back to this unfortunate point.

3.3.2. Feedback, control Lyapunov functions, stabilization.

A control Lyapunov function **(CLF)** is a function that can be made a Lyapunov function (roughly speaking, a function that decreases along all trajectories, some call this an “artificial potential”) for the closed-loop system corresponding to *some* feedback law. This can be translated into a partial differential relation sometimes called “Artstein’s (in)equation” [21]. There is a definite parallel between a CLF for stabilization, solution of this differential inequation on the one hand, and the value function of an optimal control problem for the system, solution of a HJB equation on the other hand. Now, optimal control is a quantitative objective while stabilization is a qualitative objective; it is not surprising that Artstein (in)equation is very under-determined and has many more solutions than HJB equation, and that it may (although not always) even have smooth ones.

We have, in the team, a longstanding research record on the topic of construction of CLFs and stabilizing feedback controls. This is all the more interesting as our line of research has been pointing in almost opposite directions. [36], [55], [57] insist on the construction of continuous feedback, hence smooth CLFs whereas, on the contrary, [34], [59], [60] proceed with a very fine study of non-smooth CLFs, yet good enough (semi-concave) that they can produce a reasonable discontinuous feedback with reasonable properties.

3.4. Optimal Transport

We believe that matching optimal transport with geometric control theory is one originality of our team. We expect interactions in both ways.

The study of optimal mass transport problems in the Euclidean or Riemannian setting has a long history which goes from the pioneer works of Monge [53] and Kantorovitch [46] to the recent revival initiated by fundamental contributions due to Brenier [32] and McCann [52].

Th same transportation problems in the presence of differential constraints on the set of paths —like being an admissible trajectory for a control system— is quite new. The first contributors were Ambrosio and Rigot [19] who proved the existence and uniqueness of an optimal transport map for the Monge problem associated with the squared canonical sub-Riemannian distance on the Heisenberg groups. This result was extended later by Agrachev and Lee [16], then by Figalli and Rifford [37] who showed that the Ambrosio-Rigot theorem holds indeed true on many sub-Riemannian manifolds satisfying reasonable assumptions. The problem of existence and uniqueness of an optimal transport map for the squared sub-Riemannian distance on a general complete sub-Riemannian manifold remains open; it is strictly related to the regularity of the sub-Riemannian distance in the product space, and remains a formidable challenge. Generalized notions of Ricci curvatures (bounded from below) in metric spaces have been developed recently by Lott and Villani [50] and Sturm [63], [64]. A pioneer work by Juillet [43] captured the right notion of curvature for subriemannian metric in the Heisenberg group; Agrachev and Lee [17] have elaborated on this work to define new notions of curvatures in three dimensional sub-Riemannian structures. The optimal transport approach happened to be very fruitful in this context. Many things remain to do in a more general context.

3.5. Small controls and conservative systems, averaging

Using averaging techniques to study small perturbations of integrable Hamiltonian systems dates back to H. Poincaré or earlier; it gives an approximation of the (slow) evolution of quantities that are preserved in the non-perturbed system. It is very subtle in the case of multiple periods but more elementary in the single period case, here it boils down to taking the average of the perturbation along each periodic orbit; see for instance [20], [62].

When the “perturbation” is a control, these techniques may be used after deciding how the control will depend on time and state and other quantities, for instance it may be used after applying the Pontryagin Maximum Principle as in [23], [24], [33], [41]. Without deciding the control a priori, an “average control system” may be defined as in [22].

The focus is then on studying into details this simpler “averaged” problem, that can often be described by a Riemannian metric for quadratic costs or by a Finsler metric for costs like minimum time.

This line of research stemmed out of applications to space engineering, see section 4.1 . For orbit transfer in the two-body problem, an important contribution was made by B. Bonnard, J.-B. Caillau and J. Gergaud [24] in explicitly computing the solutions of the average system obtained after applying Pontryagin Maximum Principle to minimizing a quadratic integral cost; this yields an explicit calculation of the optimal control law itself. Studying the Finsler metric issued form the time-minimal case is in progress.

NECS Project-Team

3. Research Program

3.1. Introduction

NECS team deals with Networked Control Systems. Since its foundation in 2007, the team has been addressing issues of control under imperfections and constraints deriving from the network (limited computation resources of the embedded systems, delays and errors due to communication, limited energy resources), proposing co-design strategies. The team has recently moved its focus towards general problems on *control of network systems*, which involve the analysis and control of dynamical systems with a network structure or whose operation is supported by networks. This is a research domain with substantial growth and is now recognized as a priority sector by the IEEE Control Systems Society: IEEE has started in a new journal, IEEE Transactions on Control of Network Systems, whose first issue appeared in 2014.

More in detail, the research program of NECS team is along lines described in the following sections.

3.2. Distributed estimation and data fusion in network systems

This research topic concerns distributed data combination from multiple sources (sensors) and related information fusion, to achieve more specific inference than could be achieved by using a single source (sensor). It plays an essential role in many networked applications, such as communication, networked control, monitoring, and surveillance. Distributed estimation has already been considered in the team. We wish to capitalize and strengthen these activities by focusing on integration of heterogeneous, multidimensional, and large data sets:

- Heterogeneity and large data sets. This issue constitutes a clearly identified challenge for the future. Indeed, heterogeneity comes from the fact that data are given in many forms, refer to different scales, and carry different information. Therefore, data fusion and integration will be achieved by developing new multi-perception mathematical models that can allow tracking continuous (macroscopic) and discrete (microscopic) dynamics under a unified framework while making different scales interact with each other. More precisely, many scales are considered at the same time, and they evolve following a unique fully-integrated dynamics generated by the interactions of the scales. The new multi-perception models will be integrated to forecast, estimate and broadcast useful system states in a distributed way. Targeted applications include traffic networks and navigation, and concern recent grant proposals that team has elaborated, among which the SPEEDD EU FP7 project, which has been accepted and started in February 2014 and the LOCATE-ME project, which treats pedestrian navigation.
- Multidimensionality. This issue concerns the analysis and the processing of multidimensional data, organized in multiway array, in a distributed way. Robustness of previously-developed algorithms will be studied. In particular, the issue of missing data will be taken into account. In addition, since the considered multidimensional data are generated by dynamic systems, dynamic analysis of multiway array (or tensors) will be considered. The targeted applications concern distributed detection in complex networks and distributed signal processing for collaborative networks. This topic is developed in strong collaboration with UFC (Brazil).

3.3. Networked systems and graph analysis

This is a research topic at the boundaries between graph theory and dynamical systems theory.

A first main line of research will be to study complex systems whose interactions are modeled with graphs, and to unveil the effect of the graph topology on system-theoretic properties such as observability or controllability. In particular, on-going work concerns observability of graph-based systems: after preliminary results concerning consensus systems over distance-regular graphs, the aim is to extend results to more general networks. A special focus will be on the notion of 'generic properties', namely properties which depend only on the underlying graph describing the sparsity pattern, and hold true almost surely with a random choice of the non-zero coefficients. Further work will be to explore situations in which there is the need for new notions different from the classical observability or controllability. For example, in social networks or in birds flocking the potential leader might have a goal different from classical controllability, because on the one hand he might have a goal much less ambitious than being able to drive the system to any possible state (e.g., he might want to drive everybody near its own opinion, only), and on the other hand he might have much weaker tools to construct its input (e.g., he might not know the whole system's dynamics, but only a few things, possibly that the system is linear and one row of the matrix only). Another example is the question of detectability of an unknown input under the assumption that such an input has a sparsity constraint, a question arising from the fact that a cyber-physical attack might be modeled as an input aiming at controlling the system's state, and that limitations in the capabilities of the attacker might be modeled as a sparsity constraint on the input.

A second line of research will concern graph discovery, namely algorithms aiming at reconstructing some properties of the graph (such as the number of vertices, the diameter, the degree distribution, or spectral properties such as the eigenvalues of the graph Laplacian), using some measurements of quantities related to a dynamical system associated with the graph. It will be particularly challenging to consider directed graphs, and to impose that the algorithm is anonymous, i.e., that it does not makes use of labels identifying the different agents associated with vertices.

3.4. Collaborative and distributed network control

This research line deals with the problem of designing controllers with a limited use of the network information (i.e. with restricted feedback), and with the aim to reach a pre-specified global behavior. This is in contrast to centralized controllers that use the whole system information and compute the control law at some central node. Collaborative control has already been explored in the team in connection with the underwater robot fleet, and to some extent with the source seeking problem. It remains however a certain number of challenging problems that the team wishes to address:

- Design of control with limited information, able to lead to desired global behaviors. Here the graph structure is imposed by the problem, and we aim to design the "best" possible control under such a graph constraint [0]. The team would like to explore further this research line, targeting a better understanding of possible metrics to be used as a target for optimal control design. In particular, and in connection with the traffic application, the long-standing open problem of ramp metering control under minimum information will be addressed.
- Clustering control for large networks. For large and complex systems composed of several sub-networks, feedback design is usually treated at the sub-network level, and most of the times without taking into account natural interconnections between sub-networks. The team wishes to explore new control strategies, exploiting the emergent behaviors resulting from new interconnections between the network components. This requires first to build network models operating in aggregated clusters, and then to re-formulate problems where the control can be designed using the cluster boundaries rather than individual control loops inside of each network. Examples can be found in the transportation application domain, where a significant challenge will be to obtain dynamic partitioning and clustering of heterogeneous networks in homogeneous sub-networks, and then to control the perimeter flows of the clusters to optimize the network operation.

[0] Such a problem has been previously addressed in some specific applications, particularly robot fleets, and only few recent theoretical works have initiated a more systematic system-theoretic study of sparsity-constrained system realization theory and of sparsity-constrained feedback control

3.5. Transportation networks

This is currently the main application domain of the NECS team. Several interesting problems in this area capture many of the generic networks problems described above. For example, distributed collaborative algorithms can be devised for ramp-metering control and traffic-density balancing can be achieved using consensus concepts. The team is already strongly involved in this field, both this theoretical works on traffic prediction and control, and with the Grenoble Traffic Lab platform. These activities will be continued and strengthened.

NON-A Project-Team

3. Research Program

3.1. General annihilators

Estimation is quite easy in the absence of perturbations. It becomes challenging in more realistic situations, faced to measurement noises or other unknown inputs. In our works, as well as in the founding text of *Non-A*, we have shown how our estimation techniques can successfully get rid of perturbations of the so-called *structured* type, which means the ones that can be annihilated by some linear differential operator (called the annihilator). *ALIEN* already defined such operators by integral operators, but using more general convolution operators is an alternative to be analyzed, as well as defining the "best way to kill" perturbations. Open questions are:

OQ1) Does a normal form exist for such annihilators?

OQ2) Or, at least, does there exist an adequate basis representation of the annihilator in some adequate algebra?

OQ3) And lastly, can the annihilator parameters be derived from efficient tuning rules?

The two first questions will directly impact Indicators 1 (time) and 2 (complexity), whereas the last one will impact indicator 3 (robustness).

3.2. Numerical differentiation

Estimating the derivative of a (noisy) signal with a sufficient accuracy can be seen as a key problem in domains of control and diagnosis, as well as signal and image processing. At the present stage of our research, the estimation of the n-th order time derivatives of noisy signals (including noise filtering for $n = 0$) appears as a common area for the whole project, either as a research field, or as a tool that is used both for model-based and model-free techniques. *One of the open questions is about the robustness issues (Indicator 3) with respect to the annihilator, the parameters and the numerical implementation choices.*

Two classes of techniques are considered here (**Model-based** and **Model-free**), both of them aiming at non-asymptotic estimation.

In what we call *model-based techniques*, the derivative estimation is regarded as an observation problem, which means the software-based reconstruction of unmeasured variables and, more generally, a left inversion problem [0]. This involves linear/homogeneous/nonlinear state models, including ordinary equations, systems with delays, hybrid systems with impulses or switches [0], which still has to be exploited in the finite-time and fixed-time context. Power electronics is already one of the possible applications.

Model-free techniques concern the works initiated by *ALIEN*, which rely on the only information contained in the output signal and its derivatives. The corresponding algorithms rely on our algebraic annihilation viewpoint. *One open question is: How to provide an objective comparison analysis between Model-based and Model-free estimation techniques? For this, we will only concentrate on Non-Asymptotic ones. This comparison will have to be based on the three Indicators 1 (time), 2 (complexity) and 3 (robustness).*

[0]Left invertibility deals with the question of recovering the full state of a system ("observation") together with some of its inputs ("unknown input observers"), and also refers to algebraic structural conditions.

[0]Note that hybrid dynamical systems (HDS) constitute an important field of investigation since, in this case, the discrete state can be considered as an unknown input.

3.3. Model-free control

Industry is keen on simple and powerful controllers: the tuning simplicity of the classical PID controller explains its omnipresence in industrial control systems, although its performances drop when working conditions change. The last challenge we consider is to define control techniques which, instead of using sophisticated models (the development of which may be expensive), use the information contained in the output signal and its estimated derivatives, which can be regarded as "signal-based" controllers. *Such design should take into account the Indicators 1 (time), 2 (complexity) and 3 (robustness).*

3.4. Applications

Keeping in mind that we will remain focused at developing and applying fundamental methods for non-asymptotic estimation, we intend to deal with 4 main domains of application (see the lower part of Figure 1). The Lille context offers interesting opportunities in WSAN (wireless sensor and actuator networks and, more particularly, networked robots) at Inria, as well as nano/macro machining at ENSAM. A power electronics platform will be developed in ENSEA Cergy. Last, in contact with companies, several grants, patents and collaborations are expected from the applications of $i-$PID. Each of these four application domains was presented in the *Non-A* proposal:

- Networked robots, WSAN [Lille]
- Nano/macro machining [Lille]
- Multicell chopper [Lille and Cergy]
- i-PID for industry

In the present period, we choose to give a particular focus to the first item (Networked robots), which already received some development. It can be considered as the objective 4.

These applications are described with more details below.

QUANTIC Team

3. Research Program

3.1. Hardware-efficient quantum information processing

The research activities of this section and those in next sections are done in collaboration with the permanent researchers of the future QUANTIC project-team, members of Laboratoire Pierre Aigrain, Benjamin Huard (CNRS) and François Mallet (UPMC), and of Centre Automatique et Systèmes, Pierre Rouchon (Mines Paristech). They have benefited from important scientific exchanges and collaborations with the teams of Serge Haroche, Jean-Michel Raimond and Michel Brune at Laboratoire Kastler Brossel (LKB) and Collège de France and those of Michel Devoret and Robert Schoelkopf at the department of Applied Physics of Yale University.

In this scientific program, we will explore various theoretical and experimental issues concerning protection and manipulation of quantum information. Indeed, the next, critical stage in the development of Quantum Information Processing (QIP) is most certainly the active quantum error correction (QEC). Through this stage one designs, possibly using many physical qubits, an encoded logical qubit which is protected against major decoherence channels and hence admits a significantly longer effective coherence time than a physical qubit. Reliable (fault-tolerant) computation with protected logical qubits usually comes at the expense of a significant overhead in the hardware (up to thousands of physical qubits per logical qubit). Each of the involved physical qubits still needs to satisfy the best achievable properties (coherence times, coupling strengths and tunability). More remarkably, one needs to avoid undesired interactions between various subsystems. This is going to be a major difficulty for qubits on a single chip.

The usual approach for the realization of QEC is to use many qubits to obtain a larger Hilbert space of the qubit register [72], [75]. By redundantly encoding quantum information in this Hilbert space of larger dimension one make the QEC tractable: different error channels lead to distinguishable error syndromes. There are two major drawbacks in using multi-qubit registers. The first, fundamental, drawback is that with each added physical qubit, several new decoherence channels are added. Because of the exponential increase of the Hilbert's space dimension versus the linear increase in the number of decay channels, using enough qubits, one is able to eventually protect quantum information against decoherence. However, multiplying the number of possible errors, this requires measuring more error syndromes. Note furthermore that, in general, some of these new decoherence channels can lead to correlated action on many qubits and this needs to be taken into account with extra care: in particular, such kind of non-local error channels are problematic for surface codes. The second, more practical, drawback is that it is still extremely challenging to build a register of more than on the order of 10 qubits where each of the qubits is required to satisfy near the best achieved properties: these properties include the coherence time, the coupling strengths and the tunability. Indeed, building such a register is not merely only a fabrication task but rather, one requirers to look for architectures such that, each individual qubit can be addressed and controlled independently from the others. One is also required to make sure that all the noise channels are well-controlled and uncorrelated for the QEC to be effective.

We have recently introduced a new paradigm for encoding and protecting quantum information in a quantum harmonic oscillator (e.g. a high-Q mode of a 3D superconducting cavity) instead of a multi-qubit register [4]. The infinite dimensional Hilbert space of such a system can be used to redundantly encode quantum information. The power of this idea lies in the fact that the dominant decoherence channel in a cavity is photon damping, and no more decay channels are added if we increase the number of photons we insert in the cavity. Hence, only a single error syndrome needs to be measured to identify if an error has occurred or not. Indeed, we are convinced that most early proposals on continuous variable QIP [49], [45] could be revisited taking into account the design flexibilities of Quantum Superconducting Circuits (QSC) and the new coupling regimes that are provided by these systems. In particular, we have illustrated that coupling a qubit to the cavity mode in the strong dispersive regime provides an important controllability over the Hilbert space of the cavity mode [51]. Through a recent experimental work [10], we benefit from this controllability to prepare superpositions of quasi-orthogonal coherent states, also known as Schrödinger cat states.

In this Scheme, the logical qubit is encoded in a four-component Schrödinger cat state. Continuous quantum non-demolition (QND) monitoring of a single physical observable, consisting of photon number parity, enables then the tractability of single photon jumps. We obtain therefore a first-order quantum error correcting code using only a single high-Q cavity mode (for the storage of quantum information), a single qubit (providing the non-linearity needed for controllability) and a single low-Q cavity mode (for reading out the error syndrome). As shown in Figure 1 , this leads to a significant hardware economy for realization of a protected logical qubit. Our goal here is to push these ideas towards a reliable and hardware-efficient paradigm for universal quantum computation.

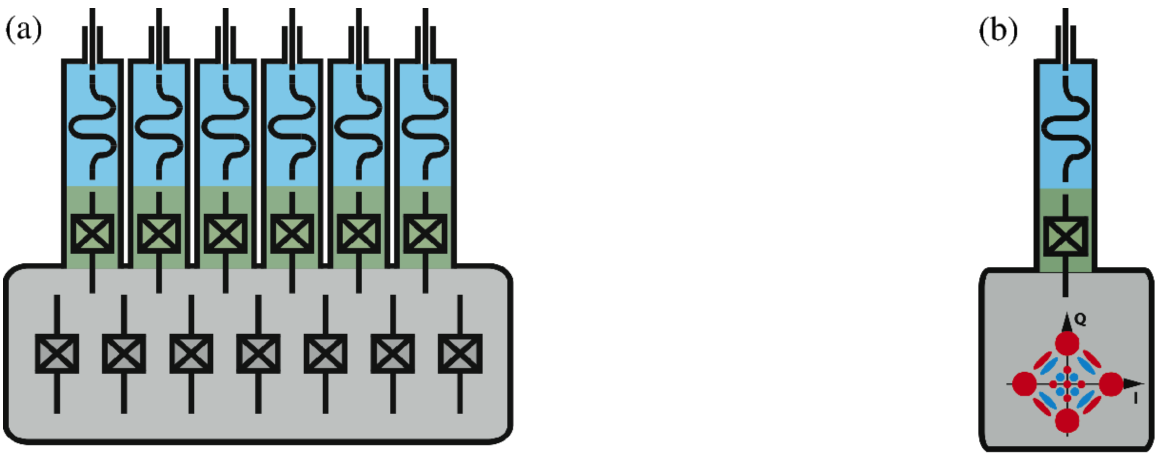


Figure 1. (a) A protected logical qubit consisting of a register of many qubits: here, we see a possible architecture for the Steane code [75] consisting of 7 qubits requiring the measurement of 6 error syndromes. In this sketch, 7 transmon qubits in a high-Q resonator and the measurement of the 6 error syndromes is ensured through 6 additional ancillary qubits with the possibility of individual readout of the ancillary qubits via independent low-Q resonators. (b) Minimal architecture for a protected logical qubit, adapted to circuit quantum electrodynamics experiments. Quantum information is encoded in a Schrödinger cat state of a single high-Q resonator mode and a single error syndrome is measured, using a single ancillary transmpn qubit and the associated readout low-Q resonator.

3.2. Reservoir (dissipation) engineering and autonomous stabilization of quantum systems

Being at the heart of any QEC protocol, the concept of feedback is central for the protection of the quantum information enabling many-qubit quantum computation or long-distance quantum communication. However, such a closed-loop control which requires a real-time and continuous measurement of the quantum system has been for long considered as counter-intuitive or even impossible. This thought was mainly caused by properties of quantum measurements: any measurement implies an instantaneous strong perturbation to the system's state. The concept of *quantum non-demolotion* (QND) measurement has played a crucial role in understanding and resolving this difficulty [30]. In the context of cavity quantum electro-dynamics (cavity QED) with Rydberg atoms [47], a first experiment on continuous QND measurements of the number of microwave photons was performed by the group at Laboratoire Kastler-Brossel (ENS) [46]. Later on, this ability of performing continuous measurements allowed the same group to realize the first continuous quantum feedback protocol stabilizing highly non-classical states of the microwave field in the cavity, the so-called photon number states [7] (this ground-breaking work was mentioned in the Nobel prize attributed to Serge Haroche). The QUANTIC team contributed to the theoretical work behind this experiment [38], [21], [74], [23]. These contributions include the development and optimization of the quantum filters taking into account the quantum measurement back-action and various measurement noises and uncertainties, the development of a feedback law based on control Lyapunov techniques, and the compensation of the feedback delay.

In the context of circuit quantum electrodynamics (circuit QED) [37], recent advances in quantum-limited amplifiers [67], [77] have opened doors to high-fidelity non-demolition measurements and real-time feedback for superconducting qubits [2]. This ability to perform high-fidelity non-demolition measurements of a quantum signal has very recently led to quantum feedback experiments with quantum superconducting circuits [77], [66], [32]. Here again, the QUANTIC team has participated to one of the first experiments in the field where the control objective is to track a dynamical trajectory of a single qubit rather than stabilizing a stationary state (this experiment was performed by the members of the future QUANTIC project-team). Such quantum trajectory tracking could be further explored to achieve metrological goals such as the stabilization of the amplitude of a microwave drive [58].

While all this progress has led to a strong optimism about the possibility to perform active protection of quantum information against decoherence, the rather short dynamical time scales of these systems limit, to a great amount, the complexity of the feedback strategies that could be employed. Indeed, in such measurement-based feedback protocols, the time-consuming data acquisition and post-treatment of the output signal leads to an important latency in the feedback procedure.

The reservoir (dissipation) engineering [64] and the closely related coherent feedback [56] are considered as alternative approaches circumventing the necessity of a real-time data acquisition, signal processing and feedback calculations. In the context of quantum information, the decoherence, caused by the coupling of a system to uncontrolled external degrees of freedom, is generally considered as the main obstacle to synthesize quantum states and to observe quantum effects. Paradoxically, it is possible to intentionally engineer a particular coupling to a reservoir in the aim of maintaining the coherence of some particular quantum states. In a general viewpoint, these approaches could be understood in the following manner: by coupling the quantum system to be stabilized to a strongly dissipative ancillary quantum system, one evacuates the entropy of the main system through the dissipation of the ancillary one. By building the feedback loop into the Hamiltonian, this type of autonomous feedback obviates the need for a complicated external control loop to correct errors. On the experimental side, such autonomous feedback techniques have been used for qubit reset [1], single-qubit state stabilization [59], and the creation [25] and stabilization [50], [55][8] of states of multipartite quantum systems.

Such reservoir engineering techniques could be widely revisited exploring the flexibility in the Hamiltonian design for QSC. We have recently developed theoretical proposals leading to extremely efficient, and simple to implement, stabilization schemes for systems consisting of a single or two qubits [1] [53]. The experimental results based on these protocols have illustrated the efficiency of the approach [1], [8]. Through these experiments, we exploit the strong dispersive interaction [70] between superconducting qubits and a single low-Q cavity mode playing the role of a dissipative reservoir. Applying some continuous-wave (cw) microwave drives with well-chosen fixed frequencies, amplitudes, and phases, we engineer an effective interaction Hamiltonian which evacuates entropy from the qubits when an eventual perturbation occurs: by driving the qubits and cavity with continuous-wave drives, we induce an autonomous feedback loop which corrects the state of the qubits every time it decays out of the desired target state. The schemes are robust against small variations of the control parameters (drives amplitudes and phase) and require only some basic calibration. Finally, by avoiding resonant interactions between the qubits and the low-Q cavity mode, the qubits remain protected against the Purcell effect, which would reduce the coherence times.

3.3. System theory for quantum information processing

In parallel and in strong interactions with the above experimental goals, we develop systematic mathematical methods for dynamical analysis, control and estimation of composite and open quantum systems. These systems are built with several quantum subsystems whose irreversible dynamics results from measurements and/or decoherence. A special attention is given to spin/spring systems made with qubits and harmonic oscillators. These developments are done in the spirit of our recent contributions [68], [21], [73], [74], [23][6] [69] resulting from collaborations with the cavity quantum electrodynamics group of Laboratoire Kastler Brossel.

3.3.1. Stabilization by measurement-based feedback

The protection of quantum information via efficient QEC is a combination of (i) tailored dynamics of a quantum system in order to protect an informational qubit from certain decoherence channels, and (ii) controlled reaction to measurements that efficiently detect and correct the dominating disturbances that are not rejected by the tailored quantum dynamics.

In such feedback scheme, the system and its measurement are quantum objects whereas the controller and the control input are classical. The stabilizing control law is based on the past values of the measurement outcomes. During our work on the LKB photon box, we have developed, for single input systems subject to quantum non-demolition measurement, a systematic stabilization method [23]: it is based on a discrete-time formulation of the dynamics, on the construction of a strict control Lyapunov function and on an explicit compensation of the feedback-loop delay. Keeping the QND measurement assumptions, extensions of such stabilization schemes will be investigated in the following directions: finite set of values for the control input with application to the convergence analysis of the atomic feedback scheme experimentally tested in [79]; multi-input case where the construction by inversion of a Metzler matrix of the strict Lyapunov function is not straightforward; continuous-time systems governed by diffusive master equations; stabilization towards a set of density operators included in a target subspace; adaptive measurement by feedback to accelerate the convergence towards a stationary state as experimentally tested in [62]. Without the QND measurement assumptions, we will also address the stabilization of non-stationary states and trajectory tracking, with applications to systems similar to those considered in [2] [32].

3.3.2. Filtering, quantum state and parameter estimations

The performance of every feedback controller crucially depends on its online estimation of the current situation. This becomes even more important for quantum systems, where full state measurements are physically impossible. Therefore the ultimate performance of feedback correction depends on fast, efficient and optimally accurate state and parameter estimations.

A quantum filter takes into account imperfection and decoherence and provides the quantum state at time $t \geq 0$ from an initial value at $t = 0$ and the measurement outcomes between 0 and t. Quantum filtering goes back to the work of Belavkin [26] and is related to quantum trajectories [34], [36]. A modern and mathematical exposure of the diffusive models is given in [24]. In [80] a first convergence analysis of diffusive filters is proposed. Nevertheless the convergence characterization and estimation of convergence rate remain open and difficult problems. For discrete time filters, a general stability result based on fidelity is proven in [68], [73]. This stability result is extended to a large class of continuous-time filters in [22]. Further efforts are required to characterize asymptotic and exponential stability. Estimations of convergence rates are available only for quantum non-demolition measurements [27]. Parameter estimations based on measurement data of quantum trajectories can be formulated within such quantum filtering framework [40], [60].

We will continue to investigate stability and convergence of quantum filtering. We will also exploit our fidelity-based stability result to justify maximum likelihood estimation and to propose, for open quantum system, parameter estimation algorithms inspired of existing estimation algorithms for classical systems. We will also investigate a more specific quantum approach: it is noticed in [31] that post-selection statistics and “past quantum” state analysis [41] enhance sensitivity to parameters and could be interesting towards increasing the precision of an estimation.

3.3.3. Stabilization by interconnections

In such stabilization schemes, the controller is also a quantum object: it is coupled to the system of interest and is subject to decoherence and thus admits an irreversible evolution. These stabilization schemes are closely related to reservoir engineering and coherent feedback [64], [56]. The closed-loop system is then a composite system built with the original system and its controller. In fact, and given our particular recent expertise in this domain [6], [1], [8], this subsection is dedicated to further developing such stabilization techniques, both experimentally and theoretically.

The main analysis issues are to prove the closed-loop convergence and to estimate the convergence rates. Since these systems are governed by Lindblad differential equations (continuous-time case) or Kraus maps (discrete-time case), their stability is automatically guaranteed: such dynamics are contractions for a large set of metrics (see [63]). Convergence and asymptotic stability is less well understood. In particular most of the convergence results consider the case where the target steady-state is a density operator of maximum rank (see, e.g., [20][chapter 4, section 6]). When the goal steady-state is not full rank very few convergence results are available.

We will focus on this geometric situation where the goal steady-state is on the boundary of the cone of positive Hermitian operators of finite trace. A specific attention will be given to adapt standard tools (Lyapunov function, passivity, contraction and Lasalle's invariance principle) for infinite dimensional systems to spin/spring structures inspired of [6], [1], [8], [5] and their associated Fokker-Planck equations for the Wigner functions.

We will also explore the Heisenberg point of view in connection with recent results of the Inria project-team MAXPLUS (algorithms and applications of algebras of max-plus type) relative to Perron-Frobenius theory [44], [43]. We will start with [71] and [65] where, based on a theorem due to Birkhoff [28], dual Lindblad equations and dual Kraus maps governing the Heisenberg evolution of any operator are shown to be contractions on the cone of Hermitian operators equipped with Hilbert's projective metric. As the Heisenberg picture is characterized by convergence of all operators to a multiple of the identity, it might provide a mean to circumvent the rank issues. We hope that such contraction tools will be especially well adapted to analyzing quantum systems composed of multiple components, motivated by the facts that the same geometry describes the contraction of classical systems undergoing synchronizing interactions [76] and by our recent generalized extension of the latter synchronizing interactions to quantum systems [57].

Besides these analysis tasks, the major challenge in stabilization by interconnections is to provide systematic methods for the design, from typical building blocks, of control systems that stabilize a specific quantum goal (state, set of states, operation) when coupled to the target system. While constructions exist for so-called linear quantum systems [61], this does not cover the states that are more interesting for quantum applications. Various strategies have been proposed that concatenate iterative control steps for open-loop steering [78], [54] with experimental limitations. The characterization of Kraus maps to stabilize any types of states has also been established [29], but without considering experimental implementations. A viable stabilization by interaction has to combine the capabilities of these various approaches, and this is a missing piece that we want to address.

3.3.3.1. Perturbation methods

With this subsection we turn towards more fundamental developments that are necessary in order to address the complexity of quantum networks with efficient reduction techniques. This should yield both efficient mathematical methods, as well as insights towards unravelling dominant physical phenomena/mechanisms in multipartite quantum dynamical systems.

In the Schrödinger point of view, the dynamics of open quantum systems are governed by master equations, either deterministic or stochastic [47], [42]. Dynamical models of composite systems are based on tensor products of Hilbert spaces and operators attached to the constitutive subsystems. Generally, a hierarchy of different timescales is present. Perturbation techniques can be very useful to construct reliable models adapted to the timescale of interest.

To eliminate high frequency oscillations possibly induced by quasi-resonant classical drives, averaging techniques are used (rotating wave approximation). These techniques are well established for closed systems without any dissipation nor irreversible effect due to measurement or decoherence. We will consider in a first step the adaptation of these averaging techniques to deterministic Lindblad master equations governing the quantum state, i.e. the system density operator. Emphasis will be put on first order and higher order corrections based on non-commutative computations with the different operators appearing in the Lindblad equations. Higher order terms could be of some interest for the protected logical qubit of figure 1 b. In future steps, we intend to explore the possibility to explicitly exploit averaging or singular perturbation properties in the design of coherent quantum feedback systems; this should be an open-systems counterpart of works like [52].

To eliminate subsystems subject to fast convergence induced by decoherence, singular perturbation techniques can be used. They provide reduced models of smaller dimension via the adiabatic elimination of the rapidly converging subsystems. The derivation of the slow dynamics is far from being obvious (see, e.g., the computations of page 142 in [33] for the adiabatic elimination of low-Q cavity). Contrarily to the classical composite systems where we have to eliminate one component in a Cartesian product, we here have to eliminate one component in a tensor product. We will adapt geometric singular perturbations [39] and invariant manifold techniques [35] to such tensor product computations to derive reduced slow approximations of any order. Such adaptations will be very useful in the context of quantum Zeno dynamics to obtain approximations of the slow dynamics on the decoherence-free subspace corresponding to the slow attractive manifold.

Perturbation methods are also precious to analyze convergence rates. Deriving the spectrum attached to the Lindblad differential equation is not obvious. We will focus on the situation where the decoherence terms of the form $L\rho L^\dagger - (L^\dagger L\rho + \rho L^\dagger L)/2$ are small compared to the conservative terms $-i[H/\hbar, \rho]$. The difficulty to overcome here is the degeneracy of the unperturbed spectrum attached to the conservative evolution $\frac{d}{dt}\rho = -i[H/\hbar, \rho]$. The degree of degeneracy of the zero eigenvalue always exceeds the dimension of the Hilbert space. Adaptations of usual perturbation techniques [48] will be investigated. They will provide estimates of convergence rates for slightly open quantum systems. We expect that such estimates will help to understand the dependance on the experimental parameters of the convergence rates observed in [1], [8] [53].

As particular outcomes for the other subsections, we expect that these developments towards simpler dominant dynamics will guide the search for optimal control strategies, both in open-loop microwave networks and in autonomous stabilization schemes such as reservoir engineering. It will further help to efficiently compute explicit convergence rates and quantitative performances for all the intended experiments.

CLASSIC Project-Team

3. Research Program

3.1. Regression models of supervised learning

The most obvious contribution of statistics to machine learning is to consider the supervised learning scenario as a special case of regression estimation: given n independent pairs of observations (X_i, Y_i), $i = 1, \cdots, n$, the aim is to "learn" the dependence of Y_i on X_i. Thus, classical results about statistical regression estimation apply, with the caveat that the hypotheses we can reasonably assume about the distribution of the pairs (X_i, Y_i) are much weaker than what is usually considered in statistical studies. The aim here is to assume very little, maybe only independence of the observed sequence of input-output pairs, and to validate model and variable selection schemes. These schemes should produce the best possible approximation of the joint distribution of (X_i, Y_i) within some restricted family of models. Their performance is evaluated according to some measure of discrepancy between distributions, a standard choice being to use the Kullback-Leibler divergence.

3.1.1. PAC-Bayes inequalities

One of the specialties of the team in this direction is to use PAC-Bayes inequalities to combine thresholded exponential moment inequalities. The name of this theory comes from its founder, David McAllester, and may be misleading. Indeed, its cornerstone is rather made of non-asymptotic entropy inequalities, and a perturbative approach to parameter estimation. The team has made major contributions to the theory, first focussed on classification [6], then on regression [1] and on principal component analysis of a random sample of points in high dimension. It has introduced the idea of combining the PAC-Bayesian approach with the use of thresholded exponential moments [7], in order to derive bounds under very weak assumptions on the noise.

DOLPHIN Project-Team

3. Research Program

3.1. Hybrid multi-objective optimization methods

The success of metaheuristics is based on their ability to find efficient solutions in a reasonable time [58]. But with very large problems and/or multi-objective problems, efficiency of metaheuristics may be compromised. Hence, in this context it is necessary to integrate metaheuristics in more general schemes in order to develop even more efficient methods. For instance, this can be done by different strategies such as cooperation and parallelization.

The DOLPHIN project deals with *"a posteriori"* multi-objective optimization where the set of Pareto solutions (solutions of best compromise) have to be generated in order to give the decision maker the opportunity to choose the solution that interests him/her.

Population-based methods, such as evolutionary algorithms, are well fitted for multi-objective problems, as they work with a set of solutions [53], [57]. To be convinced one may refer to the list of references on Evolutionary Multi-objective Optimization maintained by Carlos A. Coello [0], which contains more than 5500 references. One of the objectives of the project is to propose advanced search mechanisms for intensification and diversification. These mechanisms have been designed in an adaptive manner, since their effectiveness is related to the landscape of the MOP and to the instance solved.

In order to assess the performances of the proposed mechanisms, we always proceed in two steps: first, we carry out experiments on academic problems, for which some best known results exist; second, we use real industrial problems to cope with large and complex MOPs. The lack of references in terms of optimal or best known Pareto set is a major problem. Therefore, the obtained results in this project and the test data sets will be available at the URL http://dolphin.lille.inria.fr/ at 'benchmark'.

3.1.1. Cooperation of metaheuristics

In order to benefit from the various advantages of the different metaheuristics, an interesting idea is to combine them. Indeed, the hybridization of metaheuristics allows the cooperation of methods having complementary behaviors. The efficiency and the robustness of such methods depend on the balance between the exploration of the whole search space and the exploitation of interesting areas.

Hybrid metaheuristics have received considerable interest these last years in the field of combinatorial optimization. A wide variety of hybrid approaches have been proposed in the literature and give very good results on numerous single objective optimization problems, which are either academic (traveling salesman problem, quadratic assignment problem, scheduling problem, etc) or real-world problems. This efficiency is generally due to the combinations of single-solution based methods (iterative local search, simulated annealing, tabu search, etc) with population-based methods (genetic algorithms, ants search, scatter search, etc). A taxonomy of hybridization mechanisms may be found in [62]. It proposes to decompose these mechanisms into four classes:

- *LRH class - Low-level Relay Hybrid*: This class contains algorithms in which a given metaheuristic is embedded into a single-solution metaheuristic. Few examples from the literature belong to this class.
- *LTH class - Low-level Teamwork Hybrid*: In this class, a metaheuristic is embedded into a population-based metaheuristic in order to exploit strengths of single-solution and population-based metaheuristics.

[0] http://www.lania.mx/~ccoello/EMOO/EMOObib.html

- *HRH class - High-level Relay Hybrid*: Here, self contained metaheuristics are executed in a sequence. For instance, a population-based metaheuristic is executed to locate interesting regions and then a local search is performed to exploit these regions.
- *HTH class - High-level Teamwork Hybrid*: This scheme involves several self-contained algorithms performing a search in parallel and cooperating. An example will be the island model, based on GAs, where the population is partitioned into small subpopulations and a GA is executed per subpopulation. Some individuals can migrate between subpopulations.

Let us notice that, hybrid methods have been studied in the mono-criterion case, their application in the multi-objective context is not yet widely spread. The objective of the DOLPHIN project is to integrate specificities of multi-objective optimization into the definition of hybrid models.

3.1.2. Cooperation between metaheuristics and exact methods

Until now only few exact methods have been proposed to solve multi-objective problems. They are based either on a Branch-and-bound approach, on the algorithm $A^{\star}$, or on dynamic programming. However, these methods are limited to two objectives and, most of the time, cannot be used on a complete large scale problem. Therefore, sub search spaces have to be defined in order to use exact methods. Hence, in the same manner as hybridization of metaheuristics, the cooperation of metaheuristics and exact methods is also a main issue in this project. Indeed, it allows us to use the exploration capacity of metaheuristics, as well as the intensification ability of exact methods, which are able to find optimal solutions in a restricted search space. Sub search spaces have to be defined along the search. Such strategies can be found in the literature, but they are only applied to mono-objective academic problems.

We have extended the previous taxonomy for hybrid metaheuristics to the cooperation between exact methods and metaheuristics. Using this taxonomy, we are investigating cooperative multi-objective methods. In this context, several types of cooperations may be considered, according to the way the metaheuristic and the exact method cooperate. For instance, a metaheuristic can use an exact method for intensification or an exact method can use a metaheuristic to reduce the search space.

Moreover, a part of the DOLPHIN project deals with studying exact methods in the multi-objective context in order: i) to be able to solve small size problems and to validate proposed heuristic approaches; ii) to have more efficient/dedicated exact methods that can be hybridized with metaheuristics. In this context, the use of parallelism will push back limits of exact methods, which will be able to explore larger size search spaces [55].

3.1.3. Goals

Based on the previous works on multi-objective optimization, it appears that to improve metaheuristics, it becomes essential to integrate knowledge about the problem structure. This knowledge can be gained during the search. This would allow us to adapt operators which may be specific for multi-objective optimization or not. The goal here is to design auto-adaptive methods that are able to react to the problem structure. Moreover, regarding the hybridization and the cooperation aspects, the objectives of the DOLPHIN project are to deepen these studies as follows:

- *Design of metaheuristics for the multi-objective optimization:* To improve metaheuristics, it becomes essential to integrate knowledge about the problem structure, which we may get during the execution. This would allow us to adapt operators that may be specific for multi-objective optimization or not. The goal here is to design auto-adaptive methods that are able to react to the problem structure.
- *Design of cooperative metaheuristics:* Previous studies show the interest of hybridization for a global optimization and the importance of problem structure study for the design of efficient methods. It is now necessary to generalize hybridization of metaheuristics and to propose adaptive hybrid models that may evolve during the search while selecting the appropriate metaheuristic. Multi-objective aspects have to be introduced in order to cope with the specificities of multi-objective optimization.

- *Design of cooperative schemes between exact methods and metaheuristics:* Once the study on possible cooperation schemes is achieved, we will have to test and compare them in the multi-objective context.
- *Design and conception of parallel metaheuristics:* Our previous works on parallel metaheuristics allow us to speed up the resolution of large scale problems. It could be also interesting to study the robustness of the different parallel models (in particular in the multi-objective case) and to propose rules that determine, given a specific problem, which kind of parallelism to use. Of course these goals are not disjoined and it will be interesting to simultaneously use hybrid metaheuristics and exact methods. Moreover, those advanced mechanisms may require the use of parallel and distributed computing in order to easily make cooperating methods evolve simultaneously and to speed up the resolution of large scale problems.
- *Validation:* In order to validate the obtained results we always proceed in two phases: validation on academic problems, for which some best known results exist and use on real problems (industrial) to cope with problem size constraints.

  Moreover, those advanced mechanisms are to be used in order to integrate the distributed multi-objective aspects in the ParadisEO platform (see the paragraph on software platform).

3.2. Parallel multi-objective optimization: models and software frameworks

Parallel and distributed computing may be considered as a tool to speedup the search to solve large MOPs and to improve the robustness of a given method. Moreover, the joint use of parallelism and cooperation allows improvements on the quality of the obtained Pareto sets. Following this objective, we will design and implement parallel models for metaheuristics (evolutionary algorithms, tabu search approach) and exact methods (branch-and-bound algorithm, branch-and-cut algorithm) to solve different large MOPs.

One of the goals of the DOLPHIN project is to integrate the developed parallel models into software frameworks. Several frameworks for parallel distributed metaheuristics have been proposed in the literature. Most of them focus only either on evolutionary algorithms or on local search methods. Only few frameworks are dedicated to the design of both families of methods. On the other hand, existing optimization frameworks either do not provide parallelism at all or just supply at most one parallel model. In this project, a new framework for parallel hybrid metaheuristics is proposed, named *Parallel and Distributed Evolving Objects (ParadisEO)* based on EO. The framework provides in a transparent way the hybridization mechanisms presented in the previous section, and the parallel models described in the next section. Concerning the developed parallel exact methods for MOPs, we will integrate them into well-known frameworks such as COIN.

3.2.1. Parallel models

According to the family of addressed metaheuristics, we may distinguish two categories of parallel models: parallel models that manage a single solution, and parallel models that handle a population of solutions. The major single solution-based parallel models are the following: the *parallel neighborhood exploration model* and the *multi-start model*.

- *The parallel neighborhood exploration model* is basically a "low level" model that splits the neighborhood into partitions that are explored and evaluated in parallel. This model is particularly interesting when the evaluation of each solution is costly and/or when the size of the neighborhood is large. It has been successfully applied to the mobile network design problem (see Application section).
- *The multi-start model* consists in executing in parallel several local searches (that may be heterogeneous), without any information exchange. This model raises particularly the following question: is it equivalent to execute k local searches during a time t than executing a single local search during $k \times t$? To answer this question we tested a multi-start Tabu search on the quadratic assignment problem. The experiments have shown that the answer is often landscape-dependent. For example, the multi-start model may be well-suited for landscapes with multiple basins.

Parallel models that handle a population of solutions are mainly: the *island model*, the *central model* and *the distributed evaluation of a single solution*. Let us notice that the last model may also be used with single-solution metaheuristics.

- In *the island model*, the population is split into several sub-populations distributed among different processors. Each processor is responsible of the evolution of one sub-population. It executes all the steps of the metaheuristic from the selection to the replacement. After a given number of generations (synchronous communication), or when a convergence threshold is reached (asynchronous communication), the migration process is activated. Then, exchanges of solutions between sub-populations are realized, and received solutions are integrated into the local sub-population.
- *The central (Master/Worker) model* allows us to keep the sequentiality of the original algorithm. The master centralizes the population and manages the selection and the replacement steps. It sends sub-populations to the workers that execute the recombination and evaluation steps. The latter returns back newly evaluated solutions to the master. This approach is efficient when the generation and evaluation of new solutions is costly.
- *The distributed evaluation model* consists in a parallel evaluation of each solution. This model has to be used when, for example, the evaluation of a solution requires access to very large databases (data mining applications) that may be distributed over several processors. It may also be useful in a multi-objective context, where several objectives have to be computed simultaneously for a single solution.

As these models have now been identified, our objective is to study them in the multi-objective context in order to use them advisedly. Moreover, these models may be merged to combine different levels of parallelism and to obtain more efficient methods [56], [61].

3.2.2. Goals

Our objectives focus on these issues are the following:

- *Design of parallel models for metaheuristics and exact methods for MOPs*: We will develop parallel cooperative metaheuristics (evolutionary algorithms and local search algorithms such as the Tabu search) for solving different large MOPs. Moreover, we are designing a new exact method, named PPM (Parallel Partition Method), based on branch and bound and branch and cut algorithms. Finally, some parallel cooperation schemes between metaheuristics and exact algorithms have to be used to solve MOPs in an efficient manner.
- *Integration of the parallel models into software frameworks*: The parallel models for metaheuristics will be integrated in the ParadisEO software framework. The proposed multi-objective exact methods must be first integrated into standard frameworks for exact methods such as COIN and BOB++. A *coupling* with ParadisEO is then needed to provide hybridization between metaheuristics and exact methods.
- *Efficient deployment of the parallel models on different parallel and distributed architectures including GRIDs*: The designed algorithms and frameworks will be efficiently deployed on non-dedicated networks of workstations, dedicated cluster of workstations and SMP (Symmetric Multi-processors) machines. For GRID computing platforms, peer to peer (P2P) middlewares (XtremWeb-Condor) will be used to implement our frameworks. For this purpose, the different optimization algorithms may be re-visited for their efficient deployment.

GEOSTAT Project-Team

3. Research Program

3.1. Multiscale description in terms of multiplicative cascade

GEOSTAT is studying complex signals under the point of view of *nonlinear* methods, in the sense of *nonlinear physics* i.e. the methodologies developed to study complex systems, with a strong emphasis on multiresolution analysis. Linear methods in signal processing refer to the standard point of view under which operators are expressed by simple convolutions with impulse responses. Linear methods in signal processing are widely used, from least-square deconvolution methods in adaptive optics to source-filter models in speech processing. Because of the absence of localization of the Fourier transform, linear methods are not successful to unlock the multiscale structures and cascading properties of variables which are of primary importance as stated by the physics of the phenomena. This is the reason why new approaches, such as DFA (Detrented Fluctuation Analysis), Time-frequency analysis, variations on curvelets [56] etc. have appeared during the last decades. Recent advances in dimensionality reduction, and notably in Compressive Sensing, go beyond the Nyquist rate in sampling theory using nonlinear reconstruction, but data reduction occur at random places, independently of geometric localization of information content, which can be very useful for acquisition purposes, but of lower impact in signal analysis. One important result obtained in GEOSTAT is the effective use of multiresolution analysis associated to optimal inference along the scales of a complex system. The multiresolution analysis is performed on dimensionless quantities given by the *singularity exponents* which encode properly the geometrical structures associated to multiscale organization. This is applied successfully in the derivation of high resolution ocean dynamics, or the high resolution mapping of gaseous exchanges between the ocean and the atmosphere; the latter is of primary importance for a quantitative evaluation of global warming. Understanding the dynamics of complex systems is recognized as a new discipline, which makes use of theoretical and methodological foundations coming from nonlinear physics, the study of dynamical systems and many aspects of computer science. One of the challenges is related to the question of *emergence* in complex systems: large-scale effects measurable macroscopically from a system made of huge numbers of interactive agents [48], [45], [61], [52]. Some quantities related to nonlinearity, such as Lyapunov exponents, Kolmogorov-Sinai entropy etc. can be computed at least in the phase space [46]. Consequently, knowledge from acquisitions of complex systems (which include *complex signals*) could be obtained from information about the phase space. A result from F. Takens [57] about strange attractors in turbulence has motivated the determination of discrete dynamical systems associated to time series [50], and consequently the theoretical determination of nonlinear characteristics associated to complex acquisitions. Emergence phenomena can also be traced inside complex signals themselves, by trying to localize information content geometrically. Fundamentally, in the nonlinear analysis of complex signals there are broadly two approaches: characterization by attractors (embedding and bifurcation) and time-frequency, multiscale/multiresolution approaches. Time-frequency analysis [47] and multiscale/multiresolution are the subjects of intense research and are profoundly reshaping the analysis of complex signals by nonlinear approaches [44], [49]. In real situations, the phase space associated to the acquisition of a complex phenomenon is unknown. It is however possible to relate, inside the signal's domain, local predictability to local reconstruction and deduce from that singularity exponents (SEs) [10] [6]. The SEs are defined at any point in the signal's domain, they relate, but are different, to other kinds of exponents used in the nonlinear analysis of complex signals. We are working on their relation with:

- properties in universality classses,
- the geometric localization of multiscale properties in complex signals,
- cascading characteristics of physical variables,
- optimal wavelets and inference in multiresolution analysis.

The alternative approach taken in GEOSTAT is microscopical, or geometrical: the multiscale structures which have their "fingerprint" in complex signals are being isolated in a single realization of the complex system, i.e. using the data of the signal itself, as opposed to the consideration of grand ensembles or a wide set of realizations. This is much harder than the ergodic approaches, but it is possible because a reconstruction formula such as the one derived in [58] is local and reconstruction in the signal's domain is related to predictability. This approach is analogous to the consideration of "microcanonical ensembles" in statistical mechanics.

Nonlinear signal processing is making use of quantities related to predictability. For instance the first Lyapunov exponent λ_1 is related, from Osedelec's theorem, to the limiting behaviour of the response, after a time t, to perturbation in the phase space $\log R_\tau(t)$:

$$\lambda_1 = \lim_{t \to \infty} \frac{1}{t} \langle \log R_\tau(t) \rangle \tag{46}$$

with $\langle \cdot \rangle$ being time average and R_τ the response to a perturbation [46]. In GEOSTAT our aim is to relate such classical quantities (among others) to the behaviour of SEs, which are defined by a limiting behaviour

$$\mu\left(\mathcal{B}_r(\mathbf{x})\right) \;=\; \alpha(\mathbf{x})\, r^{d+h(\mathbf{x})} \;+\; o\left(r^{d+h(\mathbf{x})}\right) \;\; (r \to 0) \tag{47}$$

(d: dimension of the signal's domain, μ: multiscale measure, typically whose density is the gradient's norm, $\mathcal{B}_r(\mathbf{x})$: ball of radius r centered at $\mathbf{x}$). For precise computation, SEs can be smoothly interpolated by projecting wavelets:

$$\mathcal{T}_\Psi \mu(\mathbf{x}, r) = \int_{\mathbb{R}^d} \mathrm{d}\mu(\mathbf{x}') \frac{1}{r^d} \Psi\left(\frac{\mathbf{x} - \mathbf{x}'}{r}\right) \tag{48}$$

(Ψ: mother wavelet, admissible or not), but the best numerical method in computing singularity exponents lies in the definition of a measure related to predictability [16]:

$$h(\mathbf{x}) = \frac{\log \mathcal{T}_\Psi \mu(\mathbf{x}, r_0) / \langle \mathcal{T}_\Psi \mu(\cdot, r_0) \rangle}{\log r_0} + o\left(\frac{1}{\log r_0}\right) \tag{49}$$

with: r_0 is a scale choosen to diminish the amplitude of the correction term, and $\langle \mathcal{T}_\Psi \mu(\cdot, r_0) \rangle$ is the average value of the wavelet projection (mother wavelet Ψ) over the whole signal. Singularity exponents computed with this formula generalize the elementary "gradient's norm" in a very statistically coherent way across the scales.

SEs are related to the framework of reconstructible systems, and consequently to predictability. They unlock the geometric localization of a multiscale structure in a complex signal:

$$\mathcal{F}_h = \{\mathbf{x} \in \Omega \;\mid\; h(\mathbf{x}) = h\}, \tag{50}$$

(Ω: signal's domain). This multiscale structure is a fundamental feature of a complex system. Indeed, let us take the explicit example of a signal which is an acquisition of a 3D turbulent fluid. The velocity field of the flow, $\mathbf{v}(\mathbf{x}, t)$, is a solution of the Navier-Stokes equations. Fully Developped Turbulence (FDT) is defined as the regime observed when the Reynolds number $R \to \infty$, R being defined as the ratio of "viscous diffusion time" by "circulation time": $R = \frac{LV}{\nu}$,L and V being respectively characteristic length and velocity of the flow. The phase space of the associated dynamical system is infinite dimensional, while the dynamics of the flow possess one or more finite dimensional attractors. In the case of FDT, particles of the fluid in the continuum which are trapped around KAM invariant manifolds undergo random perturbations in their motion which accounts for the "boost" observed in turbulent diffusion. From there comes the observed behaviour for the energy spectrum (the law $\mathcal{E}(\mathbf{k}) \sim |\mathbf{k}|^{-5/3}$ within the inertial range), an observation that was the starting point of the Kolmogorov K41 theory, but is still not directly mathematically related from the Navier-Stokes equations. Intermittency is observed within the inertial range and is related to the fact that, in the case of FDT, symmetry is restored only in a statistical sense, a fact that has consequences on the quality of any nonlinear signal representation by frames or dictionaries.

The example of FDT as a standard "template" for developing general methods that apply to a vast class of complex systems and signals is of fundamental interest because, in FDT, the existence of a multiscale hierarchy (i.e. the collection of sets $\mathcal{F}_h$ of equation 5) which is of multifractal nature and geometrically localized can be derived from physical considerations. This geometric hierarchy of sets is responsible for the shape of the computed singularity spectra, which in turn is related to the statistical organization of information content in a signal. It explains scale invariance, a characteristic feature of complex signals. The analogy from statistical physics comes from the fact that singularity exponents are direct generalizations of *critical exponents* which explain the macroscopic properties of a system around critical points, and the quantitative characterization of *universality classes*, which allow the definition of methods and algorithms that apply to general complex signals and systems, and not only turbulent signals: signals which belong to a same universality class share common statistical organization. In GEOSTAT, the approach to singularity exponents is done within a microcanonical setting, which can interestingly be compared with other approaches such that wavelet leaders, WTMM or DFA. During the past decades, classical approaches (here called "canonical" because they use the analogy taken from the consideration of "canonical ensembles" in statistical mechanics) permitted the development of a well-established analogy taken from thermodynamics in the analysis of complex signals: if $\mathcal{F}$ is the free energy, $\mathcal{T}$ the temperature measured in energy units, $\mathcal{U}$ the internal energy per volume unit $\mathcal{S}$ the entropy and $\widehat{\beta} = 1/\mathcal{T}$, then the scaling exponents associated to moments of intensive variables $p \to \tau_p$ corresponds to $\widehat{\beta}\mathcal{F}$, $\mathcal{U}(\widehat{\beta})$ corresponds to the singularity exponents values, and $\mathcal{S}(\mathcal{U})$ to the singularity spectrum.

The singularity exponents belong to a universality class, independently of microscopic properties in the phase space of various complex systems, and beyond the particular case of turbulent data (where the existence of a multiscale hierarchy, of multifractal nature, can be inferred directly from physical considerations). They describe common multiscale statistical organizations in different complex systems [55], and this is why GEOSTAT is working on nonlinear signal processing tools that are applied to very different types of signals. The methodological framework used in GEOSTAT for analyzing complex signals is different from, but related to, the "canonical" apparatus developed in recent years (WTMM method, wavelet leaders etc.). In the microcanonical approach developed, geometrically localized singularity exponents relate to a "microcanonical" description of multiplicative cascades observed in complex systems. Indeed, it can be shown that p-dissipation at scale r associated to a fixed interval $]p, p + \Delta p[$, $\epsilon_r^{(p,\Delta p)}$, behaves in the limit $\Delta p \to 0$ as

$$\epsilon_r^{(p)} = \lim_{\Delta p \to 0} \epsilon_r^{(p,\Delta p)} = \left(\epsilon_r^{(\infty)}\right)^{h(p)/h_\infty} \tag{51}$$

which indicates the existence of a relation between the multiscale hierarchy and the geometric localization of the cascade in complex systems.

The GEOSTAT team is working particularly on the very important subject of *optimal wavelets* which are wavelets ψ that "split" the signal projections between two different scales $\mathbf{r_1} < \mathbf{r_2}$ in such a way that there exists an injection term $\zeta_{r_1/r_2}(\mathbf{x})$, independent of the process $\mathcal{T}_\psi[\mathbf{s}](\mathbf{x}, \mathbf{r})$ with:

$$\mathcal{T}_{\psi}[\mathbf{s}](\mathbf{x},\mathbf{r_1}) = \zeta_{r_1/r_2}(\mathbf{x})\mathcal{T}_{\psi}[\mathbf{s}](\mathbf{x},\mathbf{r_2}) \tag{52}$$

($\mathbf{r_1} < \mathbf{r_2}$: two scales of observation, ζ: injection variable between the scales, ψ: optimal wavelet). The **multiresolution analysis** associated to optimal wavelets is particularly interesting because it reflects, in an optimal way, the cross-scale information transfer in a complex system. These wavelets are related to persistence along the scales and lead to multiresolution analysis whose coefficients verify

$$\alpha_s = \eta_1 \alpha_f + \eta_2 \tag{53}$$

with α_s and α_f referring to child and parent coefficients, η_1 and η_2 are random variables independent of α_s and α_f and also independent of each other.

For example we give some insight about the collaboration with LEGOS Dynbio team [0] about high-resolution ocean dynamics from microcanonical formulations in nonlinear complex signal analysis. LPEs relate to the geometric structures linked with the cascading properties of indefinitely divisible variables in turbulent flows. Cascading properties can be represented by optimal wavelets (OWs); this opens new and fascinating directions of research for the determination of ocean motion field at high spatial resolution. OWs in a microcanonical sense pave the way for the determination of the energy injection mechanisms between the scales. From this results a new method for the complete evaluation of oceanic motion field; it consists in propagating along the scales the norm and the orientation of ocean dynamics deduced at low spatial resolution (geostrophic from altimetry and a part of ageostrophic from wind stress products). Using this approach, there is no need to use several temporal occurrences. Instead, the proper determination of the turbulent cascading and energy injection mechanisms in oceanographic signals allows the determination of oceanic motion field at the SST or Ocean colour spatial resolution (pixel size: 4 kms). We use the Regional Ocean Modelling System (ROMS) to validate the results on simulated data and compare the motion fields obtained with other techniques [17].

3.2. Excitable systems

Highly promising results are obtained in the application of nonlinear signal processing and multiscale techniques to the localization of heart fibrillation phenomenon acquired from a real patient and mapped over a reconstructed 3D surface of the heart. The notion of *source field*, defined in GEOSTAT from the computation of derivative measures related to the singularity exponents allows the localization of arrythmic phenomena inside the heart [7].

In speech analysis, we use the concept of the Most Singular Manifold (MSM) to localize critical events in domain of this signal. We show that in case of voiced speech signals, the MSM coincides with the instants of significant excitation of the vocal tract system. It is known that these major excitations occur when the glottis is closed, and hence, they are called the Glottal Closure Instants (GCI). We use the MSM to develop a reliable and noise robust GCI detection algorithm and we evaluate our algorithm using contemporaneous Electro-Glotto-Graph (EGG) recordings.

[0] http://www.legos.obs-mip.fr/recherches/equipes/dynbio.

MISTIS Project-Team

3. Research Program

3.1. Mixture models

Participants: Angelika Studeny, Thomas Vincent, Alexis Arnaud, Jean-Baptiste Durand, Florence Forbes, Aina Frau Pascual, Alessandro Chiancone, Stéphane Girard, Marie-José Martinez.

Key-words: mixture of distributions, EM algorithm, missing data, conditional independence, statistical pattern recognition, clustering, unsupervised and partially supervised learning.

In a first approach, we consider statistical parametric models, θ being the parameter, possibly multi-dimensional, usually unknown and to be estimated. We consider cases where the data naturally divides into observed data $y = y_1, ..., y_n$ and unobserved or missing data $z = z_1, ..., z_n$. The missing data z_i represents for instance the memberships of one of a set of K alternative categories. The distribution of an observed y_i can be written as a finite mixture of distributions,

$$f(y_i \mid \theta) = \sum_{k=1}^{K} P(z_i = k \mid \theta) f(y_i \mid z_i, \theta) \ . \tag{54}$$

These models are interesting in that they may point out hidden variable responsible for most of the observed variability and so that the observed variables are *conditionally* independent. Their estimation is often difficult due to the missing data. The Expectation-Maximization (EM) algorithm is a general and now standard approach to maximization of the likelihood in missing data problems. It provides parameter estimation but also values for missing data.

Mixture models correspond to independent z_i's. They have been increasingly used in statistical pattern recognition. They enable a formal (model-based) approach to (unsupervised) clustering.

3.2. Markov models

Participants: Angelika Studeny, Thomas Vincent, Jean-Baptiste Durand, Florence Forbes.

Key-words: graphical models, Markov properties, hidden Markov models, clustering, missing data, mixture of distributions, EM algorithm, image analysis, Bayesian inference.

Graphical modelling provides a diagrammatic representation of the dependency structure of a joint probability distribution, in the form of a network or graph depicting the local relations among variables. The graph can have directed or undirected links or edges between the nodes, which represent the individual variables. Associated with the graph are various Markov properties that specify how the graph encodes conditional independence assumptions.

It is the conditional independence assumptions that give graphical models their fundamental modular structure, enabling computation of globally interesting quantities from local specifications. In this way graphical models form an essential basis for our methodologies based on structures.

The graphs can be either directed, e.g. Bayesian Networks, or undirected, e.g. Markov Random Fields. The specificity of Markovian models is that the dependencies between the nodes are limited to the nearest neighbor nodes. The neighborhood definition can vary and be adapted to the problem of interest. When parts of the variables (nodes) are not observed or missing, we refer to these models as Hidden Markov Models (HMM). Hidden Markov chains or hidden Markov fields correspond to cases where the z_i's in (1) are distributed according to a Markov chain or a Markov field. They are a natural extension of mixture models. They are widely used in signal processing (speech recognition, genome sequence analysis) and in image processing (remote sensing, MRI, etc.). Such models are very flexible in practice and can naturally account for the phenomena to be studied.

Hidden Markov models are very useful in modelling spatial dependencies but these dependencies and the possible existence of hidden variables are also responsible for a typically large amount of computation. It follows that the statistical analysis may not be straightforward. Typical issues are related to the neighborhood structure to be chosen when not dictated by the context and the possible high dimensionality of the observations. This also requires a good understanding of the role of each parameter and methods to tune them depending on the goal in mind. Regarding estimation algorithms, they correspond to an energy minimization problem which is NP-hard and usually performed through approximation. We focus on a certain type of methods based on variational approximations and propose effective algorithms which show good performance in practice and for which we also study theoretical properties. We also propose some tools for model selection. Eventually we investigate ways to extend the standard Hidden Markov Field model to increase its modelling power.

3.3. Functional Inference, semi- and non-parametric methods

Participants: Farida Enikeeva, Alessandro Chiancone, Stéphane Girard, Gildas Mazo, Seydou-Nourou Sylla, Pablo Mesejo Santiago.

Key-words: dimension reduction, extreme value analysis, functional estimation.

We also consider methods which do not assume a parametric model. The approaches are non-parametric in the sense that they do not require the assumption of a prior model on the unknown quantities. This property is important since, for image applications for instance, it is very difficult to introduce sufficiently general parametric models because of the wide variety of image contents. Projection methods are then a way to decompose the unknown quantity on a set of functions (*e.g.* wavelets). Kernel methods which rely on smoothing the data using a set of kernels (usually probability distributions) are other examples. Relationships exist between these methods and learning techniques using Support Vector Machine (SVM) as this appears in the context of *level-sets estimation* (see section 3.3.2). Such non-parametric methods have become the cornerstone when dealing with functional data [71]. This is the case, for instance, when observations are curves. They enable us to model the data without a discretization step. More generally, these techniques are of great use for *dimension reduction* purposes (section 3.3.3). They enable reduction of the dimension of the functional or multivariate data without assumptions on the observations distribution. Semi-parametric methods refer to methods that include both parametric and non-parametric aspects. Examples include the Sliced Inverse Regression (SIR) method [74] which combines non-parametric regression techniques with parametric dimension reduction aspects. This is also the case in *extreme value analysis* [69], which is based on the modelling of distribution tails (see section 3.3.1). It differs from traditional statistics which focuses on the central part of distributions, *i.e.* on the most probable events. Extreme value theory shows that distribution tails can be modelled by both a functional part and a real parameter, the extreme value index.

3.3.1. Modelling extremal events

Extreme value theory is a branch of statistics dealing with the extreme deviations from the bulk of probability distributions. More specifically, it focuses on the limiting distributions for the minimum or the maximum of a large collection of random observations from the same arbitrary distribution. Let $X_{1,n} \leq ... \leq X_{n,n}$ denote n ordered observations from a random variable X representing some quantity of interest. A p_n-quantile of X is the value x_{p_n} such that the probability that X is greater than x_{p_n} is p_n, *i.e.*$P(X > x_{p_n}) = p_n$. When $p_n < 1/n$, such a quantile is said to be extreme since it is usually greater than the maximum observation $X_{n,n}$ (see Figure 1).

To estimate such quantiles therefore requires dedicated methods to extrapolate information beyond the observed values of X. Those methods are based on Extreme value theory. This kind of issue appeared in hydrology. One objective was to assess risk for highly unusual events, such as 100-year floods, starting from flows measured over 50 years. To this end, semi-parametric models of the tail are considered:

$$P(X > x) = x^{-1/\theta}\ell(x),\ x > x_0 > 0, \tag{55}$$

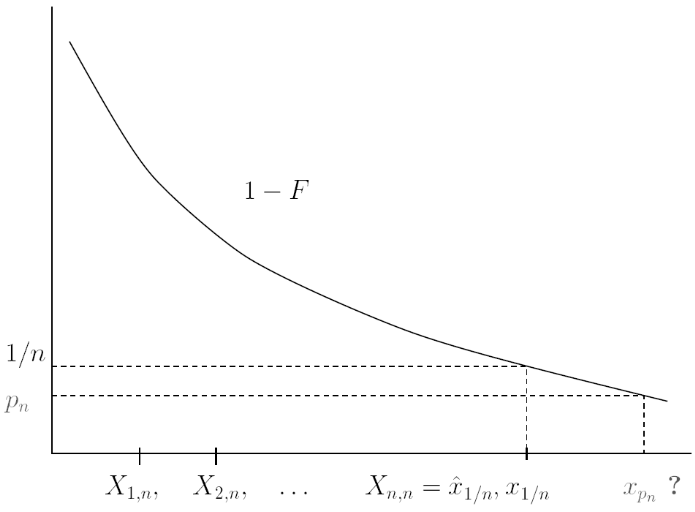


Figure 1. The curve represents the survival function $x \to P(X > x)$. The $1/n$-quantile is estimated by the maximum observation so that $\widehat{x}_{1/n} = X_{n,n}$. As illustrated in the figure, to estimate p_n-quantiles with $p_n < 1/n$, it is necessary to extrapolate beyond the maximum observation.

where both the extreme-value index $\theta > 0$ and the function $\ell(x)$ are unknown. The function ℓ is a slowly varying function *i.e.* such that

$$\frac{\ell(tx)}{\ell(x)} \to 1 \text{ as } x \to \infty \tag{56}$$

for all $t > 0$. The function $\ell(x)$ acts as a nuisance parameter which yields a bias in the classical extreme-value estimators developed so far. Such models are often referred to as heavy-tail models since the probability of extreme events decreases at a polynomial rate to zero. It may be necessary to refine the model (2 ,3) by specifying a precise rate of convergence in (3). To this end, a second order condition is introduced involving an additional parameter $\rho \leq 0$. The larger ρ is, the slower the convergence in (3) and the more difficult the estimation of extreme quantiles.

More generally, the problems that we address are part of the risk management theory. For instance, in reliability, the distributions of interest are included in a semi-parametric family whose tails are decreasing exponentially fast. These so-called Weibull-tail distributions [9] are defined by their survival distribution function:

$$P(X > x) = \exp\{-x^{\theta}\ell(x)\},\ x > x_0 > 0. \tag{57}$$

Gaussian, gamma, exponential and Weibull distributions, among others, are included in this family. An important part of our work consists in establishing links between models (2) and (4) in order to propose new estimation methods. We also consider the case where the observations were recorded with a covariate information. In this case, the extreme-value index and the p_n-quantile are functions of the covariate. We propose estimators of these functions by using moving window approaches, nearest neighbor methods, or kernel estimators.

3.3.2. Level sets estimation

Level sets estimation is a recurrent problem in statistics which is linked to outlier detection. In biology, one is interested in estimating reference curves, that is to say curves which bound 90% (for example) of the population. Points outside this bound are considered as outliers compared to the reference population. Level sets estimation can be looked at as a conditional quantile estimation problem which benefits from a non-parametric statistical framework. In particular, boundary estimation, arising in image segmentation as well as in supervised learning, is interpreted as an extreme level set estimation problem. Level sets estimation can also be formulated as a linear programming problem. In this context, estimates are sparse since they involve only a small fraction of the dataset, called the set of support vectors.

3.3.3. Dimension reduction

Our work on high dimensional data requires that we face the curse of dimensionality phenomenon. Indeed, the modelling of high dimensional data requires complex models and thus the estimation of high number of parameters compared to the sample size. In this framework, dimension reduction methods aim at replacing the original variables by a small number of linear combinations with as small as a possible loss of information. Principal Component Analysis (PCA) is the most widely used method to reduce dimension in data. However, standard linear PCA can be quite inefficient on image data where even simple image distorsions can lead to highly non-linear data. Two directions are investigated. First, non-linear PCAs can be proposed, leading to semi-parametric dimension reduction methods [72]. Another field of investigation is to take into account the application goal in the dimension reduction step. One of our approaches is therefore to develop new Gaussian models of high dimensional data for parametric inference [67]. Such models can then be used in a Mixtures or Markov framework for classification purposes. Another approach consists in combining dimension reduction, regularization techniques, and regression techniques to improve the Sliced Inverse Regression method [74].

MODAL Project-Team

3. Research Program

3.1. Generative model design

The first objective of MODAL consists in designing, analyzing, estimating and evaluating new generative parametric models for multivariate and/or heterogeneous data. It corresponds typically to continuous and categorical data but it includes also other widespread ones like ordinal, functional, ranks,...Designed models have to take into account potential correlations between variables while being (1) justifiable and realistic, (2) meaningful and parsimoniously parameterized, (3) of low computational complexity. The main purpose is to identify a few theoretical and general principles for model generation, loosely dependent on the variable nature. In this context, we propose two concurrent approaches which could be general enough for dealing with correlation between many types of homogeneous or heterogeneous variables:

- Designs general models by combining two extreme models (full dependent and full independent) which are well-defined for most of variables;
- Uses kernels as a general way for dealing with multivariate and heterogeneous variables.

3.2. Data visualization

The second objective of MODAL is to propose meaningful and quite accurate low dimensional visualizations of data typically in two-dimensional (2D) spaces, less frequently in one-dimensional (1D) or three-dimensional (3D) spaces, by using the generative models designed in the first objective. We propose also to visualize simultaneously the data and the model. All visualizations will depend on the aim at hand (typically clustering, classification or density estimation). The main originality of this objective lies in the use of models for visualization, a strategy from which we expect to have a better control on the subjectivity necessarily induced by any graphical display. In addition, the proposed approach has to be general enough to be independent on the variable nature. Note that the visualization objective is consistent with the dissemination of our methodologies through specific softwares. Indeed, displaying data is an important step in the data analysis process.

REALOPT Project-Team

3. Research Program

3.1. Introduction

Combinatorial optimization is the field of discrete optimization problems. In many applications, the most important decisions (control variables) are binary (on/off decisions) or integer (indivisible quantities). Extra variables can represent continuous adjustments or amounts. This results in models known as *mixed integer programs* (MIP), where the relationships between variables and input parameters are expressed as linear constraints and the goal is defined as a linear objective function. MIPs are notoriously difficult to solve: good quality estimations of the optimal value (bounds) are required to prune enumeration-based global-optimization algorithms whose complexity is exponential. In the standard approach to solving an MIP is so-called *branch-and-bound algorithm* : (i) one solves the linear programming (LP) relaxation using the simplex method; (ii) if the LP solution is not integer, one adds a disjunctive constraint on a factional component (rounding it up or down) that defines two sub-problems; (iii) one applies this procedure recursively, thus defining a binary enumeration tree that can be pruned by comparing the local LP bound to the best known integer solution. Commercial MIP solvers are essentially based on branch-and-bound (such IBM-CPLEX, FICO-Xpress-mp, or GUROBI). They have made tremendous progress over the last decade (with a speedup by a factor of 60). But extending their capabilities remains a continuous challenge; given the combinatorial explosion inherent to enumerative solution techniques, they remain quickly overwhelmed beyond a certain problem size or complexity.

Progress can be expected from the development of tighter formulations. Central to our field is the characterization of polyhedra defining or approximating the solution set and combinatorial algorithms to identify "efficiently" a minimum cost solution or separate an unfeasible point. With properly chosen formulations, exact optimization tools can be competitive with other methods (such as meta-heuristics) in constructing good approximate solutions within limited computational time, and of course has the important advantage of being able to provide a performance guarantee through the relaxation bounds. Decomposition techniques are implicitly leading to better problem formulation as well, while constraint propagation are tools from artificial intelligence to further improve formulation through intensive preprocessing. A new trend is robust optimization where recent progress have been made: the aim is to produce optimized solutions that remain of good quality even if the problem data has stochastic variations. In all cases, the study of specific models and challenging industrial applications is quite relevant because developments made into a specific context can become generic tools over time and see their way into commercial software.

Our project brings together researchers with expertise in mathematical programming (polyhedral approaches, Dantzig-Wolfe decomposition, mixed integer programing, robust and stochastic programming, and dynamic programming), graph theory (characterization of graph properties, combinatorial algorithms) and constraint programming in the aim of producing better quality formulations and developing new methods to exploit these formulations. These new results are then applied to find high quality solutions for practical combinatorial problems such as routing, network design, planning, scheduling, cutting and packing problems.

3.2. Polyhedral approaches for MIP

Adding valid inequalities to the polyhedral description of an MIP allows one to improve the resulting LP bound and hence to better prune the enumeration tree. In a cutting plane procedure, one attempt to identify valid inequalities that are violated by the LP solution of the current formulation and adds them to the formulation. This can be done at each node of the branch-and-bound tree giving rise to a so-called *branch-and-cut algorithm* [73]. The goal is to reduce the resolution of an integer program to that of a linear program by deriving a linear description of the convex hull of the feasible solutions. Polyhedral theory tells us that if X is a mixed integer program: $X = P \cap \mathbb{Z}^n \times \mathbb{R}^p$ where $P = \{x \in \mathbb{R}^{n+p} : Ax \leq b\}$ with matrix

$(A,b) \in \mathbb{Q}^{m\times(n+p+1)}$, then $conv(X)$ is a polyhedron that can be described in terms of linear constraints, i.e. it writes as $conv(X) = \{x \in \mathbb{R}^{n+p} : C\,x \leq d\}$ for some matrix $(C,d) \in \mathbb{Q}^{m'\times(n+p+1)}$ although the dimension m' is typically quite large. A fundamental result in this field is the equivalence of complexity between solving the combinatorial optimization problem $\min\{cx : x \in X\}$ and solving the *separation problem* over the associated polyhedron $conv(X)$: if $\widetilde{x} \notin conv(X)$, find a linear inequality $\pi\,x \geq \pi_0$ satisfied by all points in $conv(X)$ but violated by $\widetilde{x}$. Hence, for NP-hard problems, one can not hope to get a compact description of $conv(X)$ nor a polynomial time exact separation routine. Polyhedral studies focus on identifying some of the inequalities that are involved in the polyhedral description of $conv(X)$ and derive efficient *separation procedures* (cutting plane generation). Only a subset of the inequalities $C\,x \leq d$ can offer a good approximation, that combined with a branch-and-bound enumeration techniques permits to solve the problem. Using *cutting plane algorithm* at each node of the branch-and-bound tree, gives rise to the algorithm called *branch-and-cut*.

3.3. Decomposition and reformulation approaches

An hierarchical approach to tackle complex combinatorial problems consists in considering separately different substructures (subproblems). If one is able to implement relatively efficient optimization on the substructures, this can be exploited to reformulate the global problem as a selection of specific subproblem solutions that together form a global solution. If the subproblems correspond to subset of constraints in the MIP formulation, this leads to Dantzig-Wolfe decomposition. If it corresponds to isolating a subset of decision variables, this leads to Bender's decomposition. Both lead to extended formulations of the problem with either a huge number of variables or constraints. Dantzig-Wolfe approach requires specific algorithmic approaches to generate subproblem solutions and associated global decision variables dynamically in the course of the optimization. This procedure is known as *column generation*, while its combination with branch-and-bound enumeration is called *branch-and-price*. Alternatively, in Bender's approach, when dealing with exponentially many constraints in the reformulation, the *cutting plane procedures* that we defined in the previous section are well-suited tools. When optimization on a substructure is (relatively) easy, there often exists a tight reformulation of this substructure typically in an extended variable space. This gives rise powerful reformulation of the global problem, although it might be impractical given its size (typically pseudo-polynomial). It can be possible to project (part of) the extended formulation in a smaller dimensional space if not the original variable space to bring polyhedral insight (cuts derived through polyhedral studies can often be recovered through such projections).

3.4. Integration of Artificial Intelligence Techniques in Integer Programming

When one deals with combinatorial problems with a large number of integer variables, or tightly constrained problems, mixed integer programming (MIP) alone may not be able to find solutions in a reasonable amount of time. In this case, techniques from artificial intelligence can be used to improve these methods. In particular, we use primal heuristics and constraint programming.

Primal heuristics are useful to find feasible solutions in a small amount of time. We focus on heuristics that are either based on integer programming (rounding, diving, relaxation induced neighborhood search, feasibility pump), or that are used inside our exact methods (heuristics for separation or pricing subproblem, heuristic constraint propagation, ...).

Constraint Programming (CP) focuses on iteratively reducing the variable domains (sets of feasible values) by applying logical and problem-specific operators. The latter propagates on selected variables the restrictions that are implied by the other variable domains through the relations between variables that are defined by the constraints of the problem. Combined with enumeration, it gives rise to exact optimization algorithms. A CP approach is particularly effective for tightly constrained problems, feasibility problems and min-max problems Mixed Integer Programming (MIP), on the other hand, is known to be effective for loosely constrained problems and for problems with an objective function defined as the weighted sum of variables. Many problems belong to the intersection of these two classes. For such problems, it is reasonable to use algorithms that exploit complementary strengths of Constraint Programming and Mixed Integer Programming.

3.5. Robust Optimization

Decision makers are usually facing several sources of uncertainty, such as the variability in time or estimation errors. A simplistic way to handle these uncertainties is to overestimate the unknown parameters. However, this results in over-conservatism and a significant waste in resource consumption. A better approach is to account for the uncertainty directly into the decision aid model by considering mixed integer programs that involve uncertain parameters. Stochastic optimization account for the expected realization of random data and optimize an expected value representing the average situation. Robust optimization on the other hand entails protecting against the worst-case behavior of unknown data. There is an analogy to game theory where one considers an oblivious adversary choosing the realization that harms the solution the most. A full worst case protection against uncertainty is too conservative and induces very high over-cost. Instead, the realization of random data are bound to belong to a restricted feasibility set, the so-called uncertainty set. Stochastic and robust optimization rely on very large scale programs where probabilistic scenarios are enumerated. There is hope of a tractable solution for realistic size problems, provided one develops very efficient ad-hoc algorithms. The techniques for dynamically handling variables and constraints (column-and-row generation and Bender's projection tools) that are at the core of our team methodological work are specially well-suited to this context.

3.6. Polyhedral Combinatorics and Graph Theory

Many fundamental combinatorial optimization problems can be modeled as the search for a specific structure in a graph. For example, ensuring connectivity in a network amounts to building a *tree* that spans all the nodes. Inquiring about its resistance to failure amounts to searching for a minimum cardinality *cut* that partitions the graph. Selecting disjoint pairs of objects is represented by a so-called *matching*. Disjunctive choices can be modeled by edges in a so-called *conflict graph* where one searches for *stable sets* – a set of nodes that are not incident to one another. Polyhedral combinatorics is the study of combinatorial algorithms involving polyhedral considerations. Not only it leads to efficient algorithms, but also, conversely, efficient algorithms often imply polyhedral characterizations and related min-max relations. Developments of polyhedral properties of a fundamental problem will typically provide us with more interesting inequalities well suited for a branch-and-cut algorithm to more general problems. Furthermore, one can use the fundamental problems as new building bricks to decompose the more general problem at hand. For problem that let themselves easily be formulated in a graph setting, the graph theory and in particular graph decomposition theorem might help.

SELECT Project-Team

3. Research Program

3.1. General presentation

We learned from the applications we treated that some assumptions which are currently used in asymptotic theory for model selection are often irrelevant in practice. For instance, it is not realistic to assume that the target belongs to the family of models in competition. Moreover, in many situations, it is useful to make the size of the model depend on the sample size which make the asymptotic analysis breakdown. An important aim of SELECT is to propose model selection criteria which take these practical constraints into account.

3.2. A non asymptotic view for model selection

An important purpose of SELECT is to build and analyze penalized log-likelihood model selection criteria that are efficient when the number of models in competition grows to infinity with the number of observations. Concentration inequalities are a key tool for that purpose and lead to data-driven penalty choice strategies. A major issue of SELECT consists of deepening the analysis of data-driven penalties both from the theoretical and the practical side. There is no universal way of calibrating penalties but there are several different general ideas that we want to develop, including heuristics derived from the Gaussian theory, special strategies for variable selection and using resampling methods.

3.3. Taking into account the modeling purpose in model selection

Choosing a model is not only difficult theoretically. From a practical point of view, it is important to design model selection criteria that accommodate situations in which the data probability distribution P is unknown and which take the model user's purpose into account. Most standard model selection criteria assume that P belongs to one of a set of models, without considering the purpose of the model. By also considering the model user's purpose, we avoid or overcome certain theoretical difficulties and can produce flexible model selection criteria with data-driven penalties. The latter is useful in supervised Classification and hidden-structure models.

3.4. Bayesian model selection

The Bayesian approach to statistical problems is fundamentally probabilistic. A joint probability distribution is used to describe the relationships among all the unknowns and the data. Inference is then based on the posterior distribution i.e. the conditional probability distribution of the parameters given the observed data. Exploiting the internal consistency of the probability framework, the posterior distribution extracts the relevant information in the data and provides a complete and coherent summary of post-data uncertainty. Using the posterior to solve specific inference and decision problems is then straightforward, at least in principle.

SEQUEL Project-Team

3. Research Program

3.1. In Short

SEQUEL is primarily grounded on two domains:

- the problem of decision under uncertainty,
- statistical analysis and statistical learning, which provide the general concepts and tools to solve this problem.

To help the reader who is unfamiliar with these questions, we briefly present key ideas below.

3.2. Decision-making Under Uncertainty

The phrase “Decision under uncertainty” refers to the problem of taking decisions when we do not have a full knowledge neither of the situation, nor of the consequences of the decisions, as well as when the consequences of decision are non deterministic.

We introduce two specific sub-domains, namely the Markov decision processes which models sequential decision problems, and bandit problems.

3.2.1. Reinforcement Learning

Sequential decision processes occupy the heart of the SEQUEL project; a detailed presentation of this problem may be found in Puterman's book [48].

A Markov Decision Process (MDP) is defined as the tuple $(\mathcal{X}, \mathcal{A}, P, r)$ where $\mathcal{X}$ is the state space, $\mathcal{A}$ is the action space, P is the probabilistic transition kernel, and $r : \mathcal{X} \times \mathcal{A} \times \mathcal{X} \to I\!\!R$ is the reward function. For the sake of simplicity, we assume in this introduction that the state and action spaces are finite. If the current state (at time t) is $x \in \mathcal{X}$ and the chosen action is $a \in \mathcal{A}$, then the Markov assumption means that the transition probability to a new state $x' \in \mathcal{X}$ (at time $t+1$) only depends on (x, a). We write $p(x'|x, a)$ the corresponding transition probability. During a transition $(x, a) \to x'$, a reward $r(x, a, x')$ is incurred.

In the MDP $(\mathcal{X}, \mathcal{A}, P, r)$, each initial state x_0 and action sequence $a_0, a_1, ...$ gives rise to a sequence of states $x_1, x_2, ...$, satisfying $\mathbb{P}\left(x_{t+1} = x'|x_t = x, a_t = a\right) = p(x'|x, a)$, and rewards [0] $r_1, r_2, ...$ defined by $r_t = r(x_t, a_t, x_{t+1})$.

The history of the process up to time t is defined to be $H_t = (x_0, a_0, ..., x_{t-1}, a_{t-1}, x_t)$. A policy π is a sequence of functions $\pi_0, \pi_1, ...$, where π_t maps the space of possible histories at time t to the space of probability distributions over the space of actions $\mathcal{A}$. To follow a policy means that, in each time step, we assume that the process history up to time t is $x_0, a_0, ..., x_t$ and the probability of selecting an action a is equal to $\pi_t(x_0, a_0, ..., x_t)(a)$. A policy is called stationary (or Markovian) if π_t depends only on the last visited state. In other words, a policy $\pi = (\pi_0, \pi_1, ...)$ is called stationary if $\pi_t(x_0, a_0, ..., x_t) = \pi_0(x_t)$ holds for all $t \geq 0$. A policy is called deterministic if the probability distribution prescribed by the policy for any history is concentrated on a single action. Otherwise it is called a stochastic policy.

[0] Note that for simplicity, we considered the case of a deterministic reward function, but in many applications, the reward r_t itself is a random variable.

We move from an MD process to an MD problem by formulating the goal of the agent, that is what the sought policy π has to optimize? It is very often formulated as maximizing (or minimizing), in expectation, some functional of the sequence of future rewards. For example, an usual functional is the infinite-time horizon sum of discounted rewards. For a given (stationary) policy π, we define the value function $V^\pi(x)$ of that policy π at a state $x \in \mathcal{X}$ as the expected sum of discounted future rewards given that we state from the initial state x and follow the policy π:

$$V^\pi(x) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t | x_0 = x, \pi\right], \tag{58}$$

where $\mathbb{E}$ is the expectation operator and $\gamma \in (0,1)$ is the discount factor. This value function V^π gives an evaluation of the performance of a given policy π. Other functionals of the sequence of future rewards may be considered, such as the undiscounted reward (see the stochastic shortest path problems [43]) and average reward settings. Note also that, here, we considered the problem of maximizing a reward functional, but a formulation in terms of minimizing some cost or risk functional would be equivalent.

In order to maximize a given functional in a sequential framework, one usually applies Dynamic Programming (DP) [41], which introduces the optimal value function $V^*(x)$, defined as the optimal expected sum of rewards when the agent starts from a state x. We have $V^*(x) = \sup_\pi V^\pi(x)$. Now, let us give two definitions about policies:

- We say that a policy π is optimal, if it attains the optimal values $V^*(x)$ for any state $x \in \mathcal{X}$, *i.e.*, if $V^\pi(x) = V^*(x)$ for all $x \in \mathcal{X}$. Under mild conditions, deterministic stationary optimal policies exist [42]. Such an optimal policy is written π^*.
- We say that a (deterministic stationary) policy π is greedy with respect to (w.r.t.) some function V (defined on $\mathcal{X}$) if, for all $x \in \mathcal{X}$,

  $$\pi(x) \in \arg\max_{a\in\mathcal{A}} \sum_{x'\in\mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V(x')\right].$$

  where $\arg\max_{a\in\mathcal{A}} f(a)$ is the set of $a \in \mathcal{A}$ that maximizes $f(a)$. For any function V, such a greedy policy always exists because $\mathcal{A}$ is finite.

The goal of Reinforcement Learning (RL), as well as that of dynamic programming, is to design an optimal policy (or a good approximation of it).

The well-known Dynamic Programming equation (also called the Bellman equation) provides a relation between the optimal value function at a state x and the optimal value function at the successors states x' when choosing an optimal action: for all $x \in \mathcal{X}$,

$$V^*(x) = \max_{a\in\mathcal{A}} \sum_{x'\in\mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V^*(x')\right]. \tag{59}$$

The benefit of introducing this concept of optimal value function relies on the property that, from the optimal value function V^*, it is easy to derive an optimal behavior by choosing the actions according to a policy greedy w.r.t. V^*. Indeed, we have the property that a policy greedy w.r.t. the optimal value function is an optimal policy:

$$\pi^*(x) \in \arg\max_{a\in\mathcal{A}} \sum_{x'\in\mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V^*(x')\right]. \tag{60}$$

In short, we would like to mention that most of the reinforcement learning methods developed so far are built on one (or both) of the two following approaches ([54]):

- Bellman's dynamic programming approach, based on the introduction of the value function. It consists in learning a "good" approximation of the optimal value function, and then using it to derive a greedy policy w.r.t. this approximation. The hope (well justified in several cases) is that the performance V^π of the policy π greedy w.r.t. an approximation V of V^* will be close to optimality. This approximation issue of the optimal value function is one of the major challenges inherent to the reinforcement learning problem. **Approximate dynamic programming** addresses the problem of estimating performance bounds (*e.g.* the loss in performance $||V^* - V^\pi||$ resulting from using a policy π-greedy w.r.t. some approximation V- instead of an optimal policy) in terms of the approximation error $||V^* - V||$ of the optimal value function V^* by V. Approximation theory and Statistical Learning theory provide us with bounds in terms of the number of sample data used to represent the functions, and the capacity and approximation power of the considered function spaces.
- Pontryagin's maximum principle approach, based on sensitivity analysis of the performance measure w.r.t. some control parameters. This approach, also called **direct policy search** in the Reinforcement Learning community aims at directly finding a good feedback control law in a parameterized policy space without trying to approximate the value function. The method consists in estimating the so-called **policy gradient**, *i.e.* the sensitivity of the performance measure (the value function) w.r.t. some parameters of the current policy. The idea being that an optimal control problem is replaced by a parametric optimization problem in the space of parameterized policies. As such, deriving a policy gradient estimate would lead to performing a stochastic gradient method in order to search for a local optimal parametric policy.

Finally, many extensions of the Markov decision processes exist, among which the Partially Observable MDPs (POMDPs) is the case where the current state does not contain all the necessary information required to decide for sure of the best action.

3.2.2. Multi-arm Bandit Theory

Bandit problems illustrate the fundamental difficulty of decision making in the face of uncertainty: A decision maker must choose between what seems to be the best choice ("exploit"), or to test ("explore") some alternative, hoping to discover a choice that beats the current best choice.

The classical example of a bandit problem is deciding what treatment to give each patient in a clinical trial when the effectiveness of the treatments are initially unknown and the patients arrive sequentially. These bandit problems became popular with the seminal paper [49], after which they have found applications in diverse fields, such as control, economics, statistics, or learning theory.

Formally, a K-armed bandit problem ($K \geq 2$) is specified by K real-valued distributions. In each time step a decision maker can select one of the distributions to obtain a sample from it. The samples obtained are considered as rewards. The distributions are initially unknown to the decision maker, whose goal is to maximize the sum of the rewards received, or equivalently, to minimize the regret which is defined as the loss compared to the total payoff that can be achieved given full knowledge of the problem, *i.e.*, when the arm giving the highest expected reward is pulled all the time.

The name "bandit" comes from imagining a gambler playing with K slot machines. The gambler can pull the arm of any of the machines, which produces a random payoff as a result: When arm k is pulled, the random payoff is drawn from the distribution associated to k. Since the payoff distributions are initially unknown, the gambler must use exploratory actions to learn the utility of the individual arms. However, exploration has to be carefully controlled since excessive exploration may lead to unnecessary losses. Hence, to play well, the gambler must carefully balance exploration and exploitation. Auer *et al.* [40] introduced the algorithm UCB (Upper Confidence Bounds) that follows what is now called the "optimism in the face of uncertainty principle". Their algorithm works by computing upper confidence bounds for all the arms and then choosing the arm with the highest such bound. They proved that the expected regret of their algorithm increases at most at a logarithmic rate with the number of trials, and that the algorithm achieves the smallest possible regret up to some sub-logarithmic factor (for the considered family of distributions).

3.3. Statistical analysis of time series

Many of the problems of machine learning can be seen as extensions of classical problems of mathematical statistics to their (extremely) non-parametric and model-free cases. Other machine learning problems are founded on such statistical problems. Statistical problems of sequential learning are mainly those that are concerned with the analysis of time series. These problems are as follows.

3.3.1. Prediction of Sequences of Structured and Unstructured Data

Given a series of observations $x_1, \cdots, x_n$ it is required to give forecasts concerning the distribution of the future observations $x_{n+1}, x_{n+2}, \cdots$; in the simplest case, that of the next outcome x_{n+1}. Then x_{n+1} is revealed and the process continues. Different goals can be formulated in this setting. One can either make some assumptions on the probability measure that generates the sequence $x_1, \cdots, x_n, \cdots$, such as that the outcomes are independent and identically distributed (i.i.d.), or that the sequence is a Markov chain, that it is a stationary process, etc. More generally, one can assume that the data is generated by a probability measure that belongs to a certain set $\mathcal{C}$. In these cases the goal is to have the discrepancy between the predicted and the "true" probabilities to go to zero, if possible, with guarantees on the speed of convergence.

Alternatively, rather than making some assumptions on the data, one can change the goal: the predicted probabilities should be asymptotically as good as those given by the best reference predictor from a certain pre-defined set.

Another dimension of complexity in this problem concerns the nature of observations x_i. In the simplest case, they come from a finite space, but already basic applications often require real-valued observations. Moreover, function or even graph-valued observations often arise in practice, in particular in applications concerning Web data. In these settings estimating even simple characteristics of probability distributions of the future outcomes becomes non-trivial, and new learning algorithms for solving these problems are in order.

3.3.2. Hypothesis testing

Given a series of observations of $x_1, \cdots, x_n, \cdots$ generated by some unknown probability measure μ, the problem is to test a certain given hypothesis H_0 about μ, versus a given alternative hypothesis H_1. There are many different examples of this problem. Perhaps the simplest one is testing a simple hypothesis "μ is Bernoulli i.i.d. measure with probability of 0 equals 1/2" versus "μ is Bernoulli i.i.d. with the parameter different from 1/2". More interesting cases include the problems of model verification: for example, testing that μ is a Markov chain, versus that it is a stationary ergodic process but not a Markov chain. In the case when we have not one but several series of observations, we may wish to test the hypothesis that they are independent, or that they are generated by the same distribution. Applications of these problems to a more general class of machine learning tasks include the problem of feature selection, the problem of testing that a certain behaviour (such as pulling a certain arm of a bandit, or using a certain policy) is better (in terms of achieving some goal, or collecting some rewards) than another behaviour, or than a class of other behaviours.

The problem of hypothesis testing can also be studied in its general formulations: given two (abstract) hypothesis H_0 and H_1 about the unknown measure that generates the data, find out whether it is possible to test H_0 against H_1 (with confidence), and if yes then how can one do it.

3.3.3. Change Point Analysis

A stochastic process is generating the data. At some point, the process distribution changes. In the "offline" situation, the statistician observes the resulting sequence of outcomes and has to estimate the point or the points at which the change(s) occurred. In online setting, the goal is to detect the change as quickly as possible.

These are the classical problems in mathematical statistics, and probably among the last remaining statistical problems not adequately addressed by machine learning methods. The reason for the latter is perhaps in that the problem is rather challenging. Thus, most methods available so far are parametric methods concerning piecewise constant distributions, and the change in distribution is associated with the change in the mean. However, many applications, including DNA analysis, the analysis of (user) behaviour data, etc., fail to comply with this kind of assumptions. Thus, our goal here is to provide completely non-parametric methods allowing for any kind of changes in the time-series distribution.

3.3.4. Clustering Time Series, Online and Offline

The problem of clustering, while being a classical problem of mathematical statistics, belongs to the realm of unsupervised learning. For time series, this problem can be formulated as follows: given several samples $x^1 = (x_1^1, \cdots, x_{n_1}^1), \cdots, x^N = (x_N^1, \cdots, x_{n_N}^N)$, we wish to group similar objects together. While this is of course not a precise formulation, it can be made precise if we assume that the samples were generated by k different distributions.

The online version of the problem allows for the number of observed time series to grow with time, in general, in an arbitrary manner.

3.3.5. Online Semi-Supervised Learning

Semi-supervised learning (SSL) is a field of machine learning that studies learning from both labeled and unlabeled examples. This learning paradigm is extremely useful for solving real-world problems, where data is often abundant but the resources to label them are limited.

Furthermore, *online* SSL is suitable for adaptive machine learning systems. In the classification case, learning is viewed as a repeated game against a potentially adversarial nature. At each step t of this game, we observe an example $\mathbf{x_t}$, and then predict its label $\widehat{y}_t$.

The challenge of the game is that we only exceptionally observe the true label y_t. In the extreme case, which we also study, only a handful of labeled examples are provided in advance and set the initial bias of the system while unlabeled examples are gathered online and update the bias continuously. Thus, if we want to adapt to changes in the environment, we have to rely on indirect forms of feedback, such as the structure of data.

3.4. Statistical Learning and Bayesian Analysis

Before detailing some issues in these fields, let us remind the definition of a few terms.

Machine learning refers to a system capable of the autonomous acquisition and integration of knowledge. This capacity to learn from experience, analytical observation, and other means, results in a system that can continuously self-improve and thereby offer increased efficiency and effectiveness.

Statistical learning is an approach to machine intelligence that is based on statistical modeling of data. With a statistical model in hand, one applies probability theory and decision theory to get an algorithm. This is opposed to using training data merely to select among different algorithms or using heuristics/“common sense” to design an algorithm.

Bayesian Analysis applies to data that could be seen as observations in the more general meaning of the term. These data may not only come from classical sensors but also from any *device* recording information. From an operational point of view, like for statistical learning, uncertainty about the data is modeled by a probability measure thus defining the so-called likelihood functions. This last one depends upon parameters defining the state of the world we focus on for decision purposes. Within the Bayesian framework the uncertainty about these parameters is also modeled by probability measures, the priors that are subjective probabilities. Using probability theory and decision theory, one then defines new algorithms to estimate the parameters of interest and/or associated decisions. According to the International Society for Bayesian Analysis (source: http://bayesian.org), and from a more general point of view, this overall process could be summarize as follows: one assesses the current state of knowledge regarding the issue of interest, gather new data to address remaining questions, and then update and refine their understanding to incorporate both new and old data. Bayesian inference provides a logical, quantitative framework for this process based on probability theory.

Kernel method. Generally speaking, a kernel function is a function that maps a couple of points to a real value. Typically, this value is a measure of dissimilarity between the two points. Assuming a few properties on it, the kernel function implicitly defines a dot product in some function space. This very nice formal property as well as a bunch of others have ensured a strong appeal for these methods in the last 10 years in the field of function approximation. Many classical algorithms have been “kernelized”, that is, restated in a much more general way than their original formulation. Kernels also implicitly induce the representation of data in a certain “suitable” space where the problem to solve (classification, regression, ...) is expected to be simpler (non-linearity turns to linearity).

The fundamental tools used in SEQUEL come from the field of statistical learning [45]. We briefly present the most important for us to date, namely, kernel-based non parametric function approximation, and non parametric Bayesian models.

3.4.1. Non-parametric methods for Function Approximation

In statistics in general, and applied mathematics, the approximation of a multi-dimensional real function given some samples is a well-known problem (known as either regression, or interpolation, or function approximation, ...). Regressing a function from data is a key ingredient of our research, or to the least, a basic component of most of our algorithms. In the context of sequential learning, we have to regress a function while data samples are being obtained one at a time, while keeping the constraint to be able to predict points at any step along the acquisition process. In sequential decision problems, we typically have to learn a value function, or a policy.

Many methods have been proposed for this purpose. We are looking for suitable ones to cope with the problems we wish to solve. In reinforcement learning, the value function may have areas where the gradient is large; these are areas where the approximation is difficult, while these are also the areas where the accuracy of the approximation should be maximal to obtain a good policy (and where, otherwise, a bad choice of action may imply catastrophic consequences).

We particularly favor non parametric methods since they make quite a few assumptions about the function to learn. In particular, we have strong interests in l_1-regularization, and the (kernelized-)LARS algorithm. l_1-regularization yields sparse solutions, and the LARS approach produces the whole regularization path very efficiently, which helps solving the regularization parameter tuning problem.

3.4.2. Nonparametric Bayesian Estimation

Numerous problems may be solved efficiently by a Bayesian approach. The use of Monte-Carlo methods allows us to handle non–linear, as well as non–Gaussian, problems. In their standard form, they require the formulation of probability densities in a parametric form. For instance, it is a common usage to use Gaussian likelihood, because it is handy. However, in some applications such as Bayesian filtering, or blind deconvolution, the choice of a parametric form of the density of the noise is often arbitrary. If this choice is wrong, it may also have dramatic consequences on the estimation quality. To overcome this shortcoming, one possible approach is to consider that this density must also be estimated from data. A general Bayesian approach then consists in defining a probabilistic space associated with the possible outcomes of the *object* to be estimated. Applied to density estimation, it means that we need to define a probability measure on the probability density of the noise: such a measure is called a *random measure*. The classical Bayesian inference procedures can then been used. This approach being by nature non parametric, the associated frame is called *Non Parametric Bayesian*.

In particular, mixtures of Dirichlet processes [44] provide a very powerful formalism. Dirichlet Processes are a possible random measure and Mixtures of Dirichlet Processes are an extension of well-known finite mixture models. Given a mixture density $f(x|\theta)$, and $G(d\theta) = \sum_{k=1}^{\infty} \omega_k \delta_{U_k}(d\theta)$, a Dirichlet process, we define a mixture of Dirichlet processes as:

$$F(x) = \int_{\Theta} f(x|\theta) G(d\theta) = \sum_{k=1}^{\infty} \omega_k f(x|U_k) \tag{61}$$

where $F(x)$ is the density to be estimated. The class of densities that may be written as a mixture of Dirichlet processes is very wide, so that they really fit a very large number of applications.

Given a set of observations, the estimation of the parameters of a mixture of Dirichlet processes is performed by way of a Monte Carlo Markov Chain (MCMC) algorithm. Dirichlet Process Mixture are also widely used in clustering problems. Once the parameters of a mixture are estimated, they can be interpreted as the parameters of a specific cluster defining a class as well. Dirichlet processes are well known within the machine learning community and their potential in statistical signal processing still need to be developed.

3.4.3. Random Finite Sets for multisensor multitarget tracking

In the general multi-sensor multi-target Bayesian framework, an unknown (and possibly varying) number of targets whose states $x_1, ...x_n$ are observed by several sensors which produce a collection of measurements $z_1, ..., z_m$ at every time step k. Well-known models to this problem are track-based models, such as the joint probability data association (JPDA), or joint multi-target probabilities, such as the joint multi-target probability density. Common difficulties in multi-target tracking arise from the fact that the system state and the collection of measures from sensors are unordered and their size evolve randomly through time. Vector-based algorithms must therefore account for state coordinates exchanges and missing data within an unknown time interval. Although this approach is very popular and has resulted in many algorithms in the past, it may not be the optimal way to tackle the problem, since the sate and the data are in fact *sets* and not vectors.

The random finite set theory provides a powerful framework to deal with these issues. Mahler's work on finite sets statistics (FISST) provides a mathematical framework to build multi-object densities and derive the Bayesian rules for state prediction and state estimation. Randomness on object number and their states are encapsulated into random finite sets (RFS), namely multi-target(state) sets $X = \{x_1, ..., x_n\}$ and multi-sensor (measurement) set $Zk = \{z_1, ..., z_m\}$. The objective is then to propagate the multitarget probability density $f_{k|k}(X|Z(k))$ by using the Bayesian set equations at every time step k:

$$\begin{aligned} f_{k+1|k}(X|Z^{(k)}) &= \int f_{k+1|k}(X|W) f_{k|k}(W|Z^{(k)}) \delta W \\ f_{k+1|k+1}(X|Z^{(k+1)}) &= \frac{f_{k+1}(Z_{k+1}|X) f_{k+1|k}(X|Z^{(k)})}{\int f_{k+1}(Z_{k+1}|W) f_{k+1|k}(W|Z^{(k)}) \delta W} \end{aligned} \tag{62}$$

where:

- $X = \{x_1, ..., x_n\}$ is a multi-target state, *i.e.* a finite set of elements x_i defined on the single-target space $\mathcal{X}$; [0]
- $Z_{k+1} = \{z_1, ..., z_m\}$ is the current multi-sensor observation, *i.e.* a collection of measures z_i produced at time $k + 1$ by all the sensors;
- $Z^{(k)} = \bigcup_{t \leqslant k} Z_t$ is the collection of observations up to time k;
- $f_{k|k}(W|Z^{(k)})$ is the current multi-target posterior density in state W;
- $f_{k+1|k}(X|W)$ is the current multi-target Markov transition density, from state W to state X;
- $f_{k+1}(Z|X)$ is the current multi-sensor/multi-target likelihood function.

[0]The state x_i of a target is usually composed of its position, its velocity, etc.

Although equations (5) may seem similar to the classical single-sensor/single-target Bayesian equations, they are generally intractable because of the presence of the *set integrals*. For, a RFS Ξ is characterized by the family of its Janossy densities $j_{\Xi,1}(x_1)$, $j_{\Xi,2}(x_1, x_2)$... and not just by one density as it is the case with vectors. Mahler then introduced the PHD, defined on single-target state space. The PHD is the quantity whose integral on any region S is the expected number of targets inside S. Mahler proved that the PHD is the first-moment density of the multi-target probability density. Although defined on single-state space X, the PHD encapsulates information on both target number and states.

SIERRA Project-Team

3. Research Program

3.1. Supervised Learning

This part of our research focuses on methods where, given a set of examples of input/output pairs, the goal is to predict the output for a new input, with research on kernel methods, calibration methods, and multi-task learning.

3.2. Unsupervised Learning

We focus here on methods where no output is given and the goal is to find structure of certain known types (e.g., discrete or low-dimensional) in the data, with a focus on matrix factorization, statistical tests, dimension reduction, and semi-supervised learning.

3.3. Parsimony

The concept of parsimony is central to many areas of science. In the context of statistical machine learning, this takes the form of variable or feature selection. The team focuses primarily on structured sparsity, with theoretical and algorithmic contributions (this is the main topic of the ERC starting investigator grant awarded to F. Bach).

3.4. Optimization

Optimization in all its forms is central to machine learning, as many of its theoretical frameworks are based at least in part on empirical risk minimization. The team focuses primarily on convex and bandit optimization, with a particular focus on large-scale optimization.

TAO Project-Team

3. Research Program

3.1. The Four Pillars of TAO

This Section describes TAO main research directions at the crossroad of Machine Learning and Evolutionary Computation. Since 2008, TAO has been structured in several special interest groups (SIGs) to enable the agile investigation of long-term or emerging theoretical and applicative issues. The comparatively small size of TAO SIGs enables in-depth and lively discussions; the fact that all TAO members belong to several SIGs, on the basis of their personal interests, enforces the strong and informal collaboration of the groups, and the fast information dissemination.

The first two SIGs consolidate the key TAO scientific pillars, while the others evolve and adapt to new topics.

The **Stochastic Continuous Optimization** SIG (OPT-SIG) takes advantage of the fact that TAO is acknowledged the best French research group and one of the top international groups in evolutionary computation from a theoretical and algorithmic standpoint. A main priority on the OPT-SIG research agenda is to provide theoretical and algorithmic guarantees for the current world state-of-the-art continuous stochastic optimizer, CMA-ES, ranging from convergence analysis (Youhei Akimoto's post-docs) to a rigorous benchmarking methodology. Incidentally, this benchmark platform COCO has been acknowledged since 2009 as "the" international continuous optimization benchmark, and its extension is at the core of the ANR project NumBBO (started end 2012). Another priority is to address the current limitations of CMA-ES in terms of high-dimensional or expensive optimization and constraint handling (respectively Ouassim Ait El Hara's, Ilya Loshchilov's PhDs and Asma Atamna's).

The **Optimal Decision Making under Uncertainty** SIG (UCT-SIG) benefits from the MoGo expertise (see Section 5.2 and the team previous activity reports) and its past and present world records in the domain of computer-Go, establishing the international visibility of TAO in sequential decision making. Since 2010, UCT-SIG resolutely moves to address the problems of energy management from a fundamental and applied perspective. On the one hand, energy management offers a host of challenging issues, ranging from long-horizon policy optimization to the combinatorial nature of the search space, from the modeling of prior knowledge to non-stationary environment to name a few. On the other hand, the energy management issue can hardly be tackled in a pure academic perspective: tight collaborations with industrial partners are needed to access the true operational constraints. Such international and national collaborations have been started by Olivier Teytaud during his three stays (1 year, 6 months, 6 months) in Taiwan, and witnessed by the FP7 STREP Citines, the ADEME Post contract, and the METIS I-lab with SME Artelys.

The **E-Science** SIG (E-S-SIG) replaces and extends the former *Distributed systems* SIG, that was devoted to the modeling and optimization of (large scale) distributed systems, and itself was extending the goals of the original *Autonomic Computing* SIG, initiated by Cécile Germain-Renaud and investigating the use of statistical Machine Learning for large scale computational architectures, from data acquisition (the Grid Observatory in the European Grid Initiative) to grid management and fault detection. Indeed, how to model and manage network-based activities has been acknowledged a key topic *per se*, including the modeling of multi-agent systems and the exploitation of simulation results in the SimTools RNSC network frame. Further extensions are still being developped in the context of the TIMCO FUI project (started end 2012); the challenge is not only to port ML algorithms on massively distributed architectures, but to see how these architectures can inspire new ML criteria and methodologies. But these activities have become more and more application-driven, from High Energy Physics for the highly distributed computation to the Social Sciences for the multi-agents approaches – hence the change of focus of this SIG. A major result of this theme is the creation of the Paris-Saclay Center for Data Science, co-chaired by Balázs Kégl, and the organization of the Higgs-ML challenge (http://higgsml.lal.in2p3.fr/), most popular challenge ever on the Kaggle platform.

The **Designing Criteria** SIG (CRI-SIG) focuses on the design of learning and optimization criteria. It elaborates on the lessons learned from the former *Complex Systems* SIG, showing that the key issue in challenging applications often is to design the objective itself. Such targeted criteria are pervasive in the study and building of autonomous cognitive systems, ranging from intrinsic rewards in robotics to the notion of saliency in vision and image understanding. The desired criteria can also result from fundamental requirements, such as scale invariance in a statistical physics perspective, and guide the algorithmic design. Additionally, the criteria can also be domain-driven and reflect the expert priors concerning the structure of the sought solution (e.g., spatio-temporal consistency); the challenge is to formulate such criteria in a mixed convex/non differentiable objective function, amenable to tractable optimization.

The activity of the former *Crossing the Chasm* SIG gradually decreased after the completion of the 2 PhD theses funded by the Microsoft/Inria joint lab (Adapt project) and devoted to hyper-parameter tuning. As a matter of fact, though not a major research topic any more, hyper-parameter tuning has become pervasive in TAO, chiefly for continuous optimization (OPT-SIG, Section 6.3), AI planning (CRI-SIG, Section 6.5) and Air Traffic Control Optimization (Section 4.2). Recent work addressing algorithm selection using Collaborative Filtering algorithms (CRI-SIG, Section 6.5) can (and will) indeed be applied to hyper-parameter tuning for optimization algorithms.

ASPI Project-Team

3. Research Program

3.1. Interacting Monte Carlo methods and particle approximation of Feynman–Kac distributions

Monte Carlo methods are numerical methods that are widely used in situations where (i) a stochastic (usually Markovian) model is given for some underlying process, and (ii) some quantity of interest should be evaluated, that can be expressed in terms of the expected value of a functional of the process trajectory, which includes as an important special case the probability that a given event has occurred. Numerous examples can be found, e.g. in financial engineering (pricing of options and derivative securities) [36], in performance evaluation of communication networks (probability of buffer overflow), in statistics of hidden Markov models (state estimation, evaluation of contrast and score functions), etc. Very often in practice, no analytical expression is available for the quantity of interest, but it is possible to simulate trajectories of the underlying process. The idea behind Monte Carlo methods is to generate independent trajectories of this process or of an alternate instrumental process, and to build an approximation (estimator) of the quantity of interest in terms of the weighted empirical probability distribution associated with the resulting independent sample. By the law of large numbers, the above estimator converges as the size N of the sample goes to infinity, with rate $1/\sqrt{N}$ and the asymptotic variance can be estimated using an appropriate central limit theorem. To reduce the variance of the estimator, many variance reduction techniques have been proposed. Still, running independent Monte Carlo simulations can lead to very poor results, because trajectories are generated *blindly*, and only afterwards are the corresponding weights evaluated. Some of the weights can happen to be negligible, in which case the corresponding trajectories are not going to contribute to the estimator, i.e. computing power has been wasted.

A recent and major breakthrough, has been the introduction of interacting Monte Carlo methods, also known as sequential Monte Carlo (SMC) methods, in which a whole (possibly weighted) sample, called *system of particles*, is propagated in time, where the particles

- *explore* the state space under the effect of a *mutation* mechanism which mimics the evolution of the underlying process,
- and are *replicated* or *terminated*, under the effect of a *selection* mechanism which automatically concentrates the particles, i.e. the available computing power, into regions of interest of the state space.

In full generality, the underlying process is a discrete–time Markov chain, whose state space can be

> finite, continuous, hybrid (continuous / discrete), graphical, constrained, time varying, pathwise, etc.,

the only condition being that it can easily be *simulated*.

In the special case of particle filtering, originally developed within the tracking community, the algorithms yield a numerical approximation of the optimal Bayesian filter, i.e. of the conditional probability distribution of the hidden state given the past observations, as a (possibly weighted) empirical probability distribution of the system of particles. In its simplest version, introduced in several different scientific communities under the name of *bootstrap filter* [38], *Monte Carlo filter* [43] or *condensation* (conditional density propagation) algorithm [40], and which historically has been the first algorithm to include a redistribution step, the selection mechanism is governed by the likelihood function: at each time step, a particle is more likely to survive and to replicate at the next generation if it is consistent with the current observation. The algorithms also provide as a by–product a numerical approximation of the likelihood function, and of many other contrast functions for parameter estimation in hidden Markov models, such as the prediction error or the conditional least–squares criterion.

Particle methods are currently being used in many scientific and engineering areas

> positioning, navigation, and tracking [39], [33], visual tracking [40], mobile robotics [34], [55], ubiquitous computing and ambient intelligence, sensor networks, risk evaluation and simulation of rare events [37], genetics, molecular simulation [35], etc.

Other examples of the many applications of particle filtering can be found in the contributed volume [22] and in the special issue of *IEEE Transactions on Signal Processing* devoted to *Monte Carlo Methods for Statistical Signal Processing* in February 2002, where the tutorial paper [23] can be found, and in the textbook [52] devoted to applications in target tracking. Applications of sequential Monte Carlo methods to other areas, beyond signal and image processing, e.g. to genetics, can be found in [51]. A recent overview can also be found in [25].

Particle methods are very easy to implement, since it is sufficient in principle to simulate independent trajectories of the underlying process. The whole problematic is multidisciplinary, not only because of the already mentioned diversity of the scientific and engineering areas in which particle methods are used, but also because of the diversity of the scientific communities which have contributed to establish the foundations of the field

> target tracking, interacting particle systems, empirical processes, genetic algorithms (GA), hidden Markov models and nonlinear filtering, Bayesian statistics, Markov chain Monte Carlo (MCMC) methods.

These algorithms can be interpreted as numerical approximation schemes for Feynman–Kac distributions, a pathwise generalization of Gibbs–Boltzmann distributions, in terms of the weighted empirical probability distribution associated with a system of particles. This abstract point of view [31], [29], has proved to be extremely fruitful in providing a very general framework to the design and analysis of numerical approximation schemes, based on systems of branching and / or interacting particles, for nonlinear dynamical systems with values in the space of probability distributions, associated with Feynman–Kac distributions. Many asymptotic results have been proved as the number N of particles (sample size) goes to infinity, using techniques coming from applied probability (interacting particle systems, empirical processes [56]), see e.g. the survey article [31] or the textbooks [29], [28], and references therein

> convergence in ^{p}, convergence as empirical processes indexed by classes of functions, uniform convergence in time, see also [48], [49], central limit theorem, see also [45], propagation of chaos, large deviations principle, etc.

The objective here is to systematically study the impact of the many algorithmic variants on the convergence results.

3.2. Statistics of HMM

Hidden Markov models (HMM) form a special case of partially observed stochastic dynamical systems, in which the state of a Markov process (in discrete or continuous time, with finite or continuous state space) should be estimated from noisy observations. The conditional probability distribution of the hidden state given past observations is a well–known example of a normalized (nonlinear) Feynman–Kac distribution, see 3.1 . These models are very flexible, because of the introduction of latent variables (non observed) which allows to model complex time dependent structures, to take constraints into account, etc. In addition, the underlying Markovian structure makes it possible to use numerical algorithms (particle filtering, Markov chain Monte Carlo methods (MCMC), etc.) which are computationally intensive but whose complexity is rather small. Hidden Markov models are widely used in various applied areas, such as speech recognition, alignment of biological sequences, tracking in complex environment, modeling and control of networks, digital communications, etc.

Beyond the recursive estimation of a hidden state from noisy observations, the problem arises of statistical inference of HMM with general state space [26], including estimation of model parameters, early monitoring and diagnosis of small changes in model parameters, etc.

Large time asymptotics A fruitful approach is the asymptotic study, when the observation time increases to infinity, of an extended Markov chain, whose state includes (i) the hidden state, (ii) the observation, (iii) the prediction filter (i.e. the conditional probability distribution of the hidden state given observations at all previous time instants), and possibly (iv) the derivative of the prediction filter with respect to the parameter. Indeed, it is easy to express the log–likelihood function, the conditional least–squares criterion, and many other clasical contrast processes, as well as their derivatives with respect to the parameter, as additive functionals of the extended Markov chain.

The following general approach has been proposed

- first, prove an exponential stability property (i.e. an exponential forgetting property of the initial condition) of the prediction filter and its derivative, for a misspecified model,
- from this, deduce a geometric ergodicity property and the existence of a unique invariant probability distribution for the extended Markov chain, hence a law of large numbers and a central limit theorem for a large class of contrast processes and their derivatives, and a local asymptotic normality property,
- finally, obtain the consistency (i.e. the convergence to the set of minima of the associated contrast function), and the asymptotic normality of a large class of minimum contrast estimators.

This programme has been completed in the case of a finite state space [7], and has been generalized [32] under an uniform minoration assumption for the Markov transition kernel, which typically does only hold when the state space is compact. Clearly, the whole approach relies on the existence of an exponential stability property of the prediction filter, and the main challenge currently is to get rid of this uniform minoration assumption for the Markov transition kernel [30], [49], so as to be able to consider more interesting situations, where the state space is noncompact.

Small noise asymptotics Another asymptotic approach can also be used, where it is rather easy to obtain interesting explicit results, in terms close to the language of nonlinear deterministic control theory [44]. Taking the simple example where the hidden state is the solution to an ordinary differential equation, or a nonlinear state model, and where the observations are subject to additive Gaussian white noise, this approach consists in assuming that covariances matrices of the state noise and of the observation noise go simultaneously to zero. If it is reasonable in many applications to consider that noise covariances are small, this asymptotic approach is less natural than the large time asymptotics, where it is enough (provided a suitable ergodicity assumption holds) to accumulate observations and to see the expected limit laws (law of large numbers, central limit theorem, etc.). In opposition, the expressions obtained in the limit (Kullback–Leibler divergence, Fisher information matrix, asymptotic covariance matrix, etc.) take here a much more explicit form than in the large time asymptotics.

The following results have been obtained using this approach

- the consistency of the maximum likelihood estimator (i.e. the convergence to the set M of global minima of the Kullback–Leibler divergence), has been obtained using large deviations techniques, with an analytical approach [41],
- if the abovementioned set M does not reduce to the true parameter value, i.e. if the model is not identifiable, it is still possible to describe precisely the asymptotic behavior of the estimators [42]: in the simple case where the state equation is a noise–free ordinary differential equation and using a Bayesian framework, it has been shown that (i) if the rank r of the Fisher information matrix I is constant in a neighborhood of the set M, then this set is a differentiable submanifold of codimension r, (ii) the posterior probability distribution of the parameter converges to a random probability distribution in the limit, supported by the manifold M, absolutely continuous w.r.t. the Lebesgue measure on M, with an explicit expression for the density, and (iii) the posterior probability distribution of the suitably normalized difference between the parameter and its projection on the manifold M, converges to a mixture of Gaussian probability distributions on the normal spaces to the manifold M, which generalized the usual asymptotic normality property,

- it has been shown [50] that (i) the parameter dependent probability distributions of the observations are locally asymptotically normal (LAN) [47], from which the asymptotic normality of the maximum likelihood estimator follows, with an explicit expression for the asymptotic covariance matrix, i.e. for the Fisher information matrix I, in terms of the Kalman filter associated with the linear tangent linear Gaussian model, and (ii) the score function (i.e. the derivative of the log–likelihood function w.r.t. the parameter), evaluated at the true value of the parameter and suitably normalized, converges to a Gaussian r.v. with zero mean and covariance matrix I.

3.3. Multilevel splitting for rare event simulation

See 4.2 , and 5.1 , 5.2 , and 5.3 .

The estimation of the small probability of a rare but critical event, is a crucial issue in industrial areas such as

> nuclear power plants, food industry, telecommunication networks, finance and insurance industry, air traffic management, etc.

In such complex systems, analytical methods cannot be used, and naive Monte Carlo methods are clearly unefficient to estimate accurately very small probabilities. Besides importance sampling, an alternate widespread technique consists in multilevel splitting [46], where trajectories going towards the critical set are given offsprings, thus increasing the number of trajectories that eventually reach the critical set. As shown in [5], the Feynman–Kac formalism of 3.1 is well suited for the design and analysis of splitting algorithms for rare event simulation.

Propagation of uncertainty Multilevel splitting can be used in static situations. Here, the objective is to learn the probability distribution of an output random variable $Y=F(X)$, where the function F is only defined pointwise for instance by a computer programme, and where the probability distribution of the input random variable X is known and easy to simulate from. More specifically, the objective could be to compute the probability of the output random variable exceeding a threshold, or more generally to evaluate the cumulative distribution function of the output random variable for different output values. This problem is characterized by the lack of an analytical expression for the function, the computational cost of a single pointwise evaluation of the function, which means that the number of calls to the function should be limited as much as possible, and finally the complexity and / or unavailability of the source code of the computer programme, which makes any modification very difficult or even impossible, for instance to change the model as in importance sampling methods.

The key issue is to learn as fast as possible regions of the input space which contribute most to the computation of the target quantity. The proposed splitting methods consists in (i) introducing a sequence of intermediate regions in the input space, implicitly defined by exceeding an increasing sequence of thresholds or levels, (ii) counting the fraction of samples that reach a level given that the previous level has been reached already, and (iii) improving the diversity of the selected samples, usually using an artificial Markovian dynamics. In this way, the algorithm learns

- the transition probability between successive levels, hence the probability of reaching each intermediate level,
- and the probability distribution of the input random variable, conditionned on the output variable reaching each intermediate level.

A further remark, is that this conditional probability distribution is precisely the optimal (zero variance) importance distribution needed to compute the probability of reaching the considered intermediate level.

Rare event simulation To be specific, consider a complex dynamical system modelled as a Markov process, whose state can possibly contain continuous components and finite components (mode, regime, etc.), and the objective is to compute the probability, hopefully very small, that a critical region of the state space is reached by the Markov process before a final time T, which can be deterministic and fixed, or random (for instance the time of return to a recurrent set, corresponding to a nominal behaviour).

The proposed splitting method consists in (i) introducing a decreasing sequence of intermediate, more and more critical, regions in the state space, (ii) counting the fraction of trajectories that reach an intermediate region before time T, given that the previous intermediate region has been reached before time T, and (iii) regenerating the population at each stage, through redistribution. In addition to the non–intrusive behaviour of the method, the splitting methods make it possible to learn the probability distribution of typical critical trajectories, which reach the critical region before final time T, an important feature that methods based on importance sampling usually miss. Many variants have been proposed, whether

- the branching rate (number of offsprings allocated to a successful trajectory) is fixed, which allows for depth–first exploration of the branching tree, but raises the issue of controlling the population size,
- the population size is fixed, which requires a breadth–first exploration of the branching tree, with random (multinomial) or deterministic allocation of offsprings, etc.

Just as in the static case, the algorithm learns

- the transition probability between successive levels, hence the probability of reaching each intermediate level,
- and the entrance probability distribution of the Markov process in each intermediate region.

Contributions have been given to

- minimizing the asymptotic variance, obtained through a central limit theorem, with respect to the shape of the intermediate regions (selection of the importance function), to the thresholds (levels), to the population size, etc.
- controlling the probability of extinction (when not even one trajectory reaches the next intermediate level),
- designing and studying variants suited for hybrid state space (resampling per mode, marginalization, mode aggregation),

and in the static case, to

- minimizing the asymptotic variance, obtained through a central limit theorem, with respect to intermediate levels, to the Metropolis kernel introduced in the mutation step, etc.

A related issue is global optimization. Indeed, the difficult problem of finding the set M of global minima of a real–valued function V can be replaced by the apparently simpler problem of sampling a population from a probability distribution depending on a small parameter, and asymptotically supported by the set M as the small parameter goes to zero. The usual approach here is to use the cross–entropy method [53], [27], which relies on learning the optimal importance distribution within a prescribed parametric family. On the other hand, multilevel splitting methods could provide an alternate nonparametric approach to this problem.

3.4. Nearest neighbor estimates

This additional topic was not present in the initial list of objectives, and has emerged only recently.

In pattern recognition and statistical learning, also known as machine learning, nearest neighbor (NN) algorithms are amongst the simplest but also very powerful algorithms available. Basically, given a training set of data, i.e. an N–sample of i.i.d. object–feature pairs, with real–valued features, the question is how to generalize, that is how to guess the feature associated with any new object. To achieve this, one chooses some integer k smaller than N, and takes the mean–value of the k features associated with the k objects that are nearest to the new object, for some given metric.

In general, there is no way to guess exactly the value of the feature associated with the new object, and the minimal error that can be done is that of the Bayes estimator, which cannot be computed by lack of knowledge of the distribution of the object–feature pair, but the Bayes estimator can be useful to characterize the strength of the method. So the best that can be expected is that the NN estimator converges, say when the sample size N grows, to the Bayes estimator. This is what has been proved in great generality by Stone [54] for the mean square convergence, provided that the object is a finite–dimensional random variable, the feature is a square–integrable random variable, and the ratio k/N goes to 0. Nearest neighbor estimator is not the only local averaging estimator with this property, but it is arguably the simplest.

The asymptotic behavior when the sample size grows is well understood in finite dimension, but the situation is radically different in general infinite dimensional spaces, when the objects to be classified are functions, images, etc.

Nearest neighbor classification in infinite dimension In finite dimension, the k–nearest neighbor classifier is universally consistent, i.e. its probability of error converges to the Bayes risk as N goes to infinity, whatever the joint probability distribution of the pair, provided that the ratio k/N goes to zero. Unfortunately, this result is no longer valid in general metric spaces, and the objective is to find out reasonable sufficient conditions for the weak consistency to hold. Even in finite dimension, there are exotic distances such that the nearest neighbor does not even get closer (in the sense of the distance) to the point of interest, and the state space needs to be complete for the metric, which is the first condition. Some regularity on the regression function is required next. Clearly, continuity is too strong because it is not required in finite dimension, and a weaker form of regularity is assumed. The following consistency result has been obtained: if the metric space is separable and if some Besicovich condition holds, then the nearest neighbor classifier is weakly consistent. Note that the Besicovich condition is always fulfilled in finite dimensional vector spaces (this result is called the Besicovich theorem), and that a counterexample [3] can be given in an infinite dimensional space with a Gaussian measure (in this case, the nearest neighbor classifier is clearly nonconsistent). Finally, a simple example has been found which verifies the Besicovich condition with a noncontinuous regression function.

Rates of convergence of the functional k–nearest neighbor estimator Motivated by a broad range of potential applications, such as regression on curves, rates of convergence of the k–nearest neighbor estimator of the regression function, based on N independent copies of the object–feature pair, have been investigated when the object is in a suitable ball in some functional space. Using compact embedding theory, explicit and general finite sample bounds can be obtained for the expected squared difference between the k–nearest neighbor estimator and the Bayes regression function, in a very general setting. The results have also been particularized to classical function spaces such as Sobolev spaces, Besov spaces and reproducing kernel Hilbert spaces. The rates obtained are genuine nonparametric convergence rates, and up to our knowledge the first of their kind for k–nearest neighbor regression.

This emerging topic has produced several theoretical advances [1], [2] in collaboration with Gérard Biau (université Pierre et Marie Curie, ENS Paris and EPI CLASSIC, Inria Paris—Rocquencourt), and a possible target application domain has been identified in the statistical analysis of recommendation systems, that would be a source of interesting problems.

CQFD Project-Team

3. Research Program

3.1. Introduction

The scientific objectives of the team are to provide mathematical tools for modeling and optimization of complex systems. These systems require mathematical representations which are in essence dynamic, multi-model and stochastic. This increasing complexity poses genuine scientific challenges in the domain of modeling and optimization. More precisely, our research activities are focused on stochastic optimization and (parametric, semi-parametric, multidimensional) statistics which are complementary and interlinked topics. It is essential to develop simultaneously statistical methods for the estimation and control methods for the optimization of the models.

3.2. Main research topics

- Stochastic modeling: Markov chain, Piecewise Deterministic Markov Processes (PDMP), Markov Decision Processes (MDP).
  The mathematical representation of complex systems is a preliminary step to our final goal corresponding to the optimization of its performance. For example, in order to optimize the predictive maintenance of a system, it is necessary to choose the adequate model for its representation. The step of modeling is crucial before any estimation or computation of quantities related to its optimization. For this we have to represent all the different regimes of the system and the behavior of the physical variables under each of these regimes. Moreover, we must also select the dynamic variables which have a potential effect on the physical variable and the quantities of interest. The team CQFD works on the theory of Piecewise Deterministic Markov Processes (PDMP's) and on Markov Decision Processes (MDP's). These two classes of systems form general families of controlled stochastic processes suitable for the modeling of sequential decision-making problems in the continuous-time (PDMPs) and discrete-time (MDP's) context. They appear in many fields such as engineering, computer science, economics, operations research and constitute powerful class of processes for the modeling of complex system.
- Estimation methods: estimation for PDMP; estimation in non- and semi parametric regression modeling.
  To the best of our knowledge, there does not exist any general theory for the problems of estimating parameters of PDMPs although there already exist a large number of tools for sub-classes of PDMPs such as point processes and marked point processes. However, to fill the gap between these specific models and the general class of PDMPs, new theoretical and mathematical developments will be on the agenda of the whole team. In the framework of non-parametric regression or quantile regression, we focus on kernel estimators or kernel local linear estimators for complete data or censored data. New strategies for estimating semi-parametric models via recursive estimation procedures have also received an increasing interest recently. The advantage of the recursive estimation approach is to take into account the successive arrivals of the information and to refine, step after step, the implemented estimation algorithms. These recursive methods do require restarting calculation of parameter estimation from scratch when new data are added to the base. The idea is to use only the previous estimations and the new data to refresh the estimation. The gain in time could be very interesting and there are many applications of such approaches.

- Dimension reduction: dimension-reduction via SIR and related methods, dimension-reduction via multidimensional and classification methods.
  Most of the dimension reduction approaches seek for lower dimensional subspaces minimizing the loss of some statistical information. This can be achieved in modeling framework or in exploratory data analysis context.
  In modeling framework we focus our attention on semi-parametric models in order to conjugate the advantages of parametric and nonparametric modeling. On the one hand, the parametric part of the model allows a suitable interpretation for the user. On the other hand, the functional part of the model offers a lot of flexibility. In this project, we are especially interested in the semi-parametric regression model $Y = f(X'\theta) + \varepsilon$, the unknown parameter θ belongs to $\mathbb{R}^p$ for a single index model, or is such that $\theta = [\theta_1, \cdots, \theta_d]$ (where each θ_k belongs to $\mathbb{R}^p$ and $d \leq p$ for a multiple indices model), the noise ε is a random error with unknown distribution, and the link function f is an unknown real valued function. Another way to see this model is the following: the variables X and Y are independent given $X'\theta$. In our semi-parametric framework, the main objectives are to estimate the parametric part θ as well as the nonparametric part which can be the link function f, the conditional distribution function of Y given X or the conditional quantile q_α. In order to estimate the dimension reduction parameter θ we focus on the Sliced Inverse Regression (SIR) method which has been introduced by Li [57] and Duan and Li [55]
  Methods of dimension reduction are also important tools in the field of data analysis, data mining and machine learning.They provide a way to understand and visualize the structure of complex data sets.Traditional methods among others are principal component analysis for quantitative variables or multiple component analysis for qualitative variables. New techniques have also been proposed to address these challenging tasks involving many irrelevant and redundant variables and often comparably few observation units. In this context, we focus on the problem of synthetic variables construction, whose goals include increasing the predictor performance and building more compact variables subsets. Clustering of variables is used for feature construction. The idea is to replace a group of ”similar” variables by a cluster centroid, which becomes a feature. The most popular algorithms include K-means and hierarchical clustering. For a review, see, e.g., the textbook of Duda [56]
- Stochastic optimal control: optimal stopping, impulse control, continuous control, linear programming.
  The first objective is to focus on the development of computational methods.
  - In the continuous-time context, stochastic control theory has from the numerical point of view, been mainly concerned with Stochastic Differential Equations (SDEs in short). From the practical and theoretical point of view, the numerical developments for this class of processes are extensive and largely complete. It capitalizes on the connection between SDEs and second order partial differential equations (PDEs in short) and the fact that the properties of the latter equations are very well understood. It is, however, hard to deny that the development of computational methods for the control of PDMPs has received little attention. One of the main reasons is that the role played by the familiar PDEs in the diffusion models is here played by certain systems of integro-differential equations for which there is not (and cannot be) a unified theory such as for PDEs as emphasized by M.H.A. Davis in his book. To the best knowledge of the team, there is only one attempt to tackle this difficult problem by O.L.V. Costa and M.H.A. Davis. The originality of our project consists in studying this unexplored area. It is very important to stress the fact that these numerical developments will give rise to a lot of theoretical issues such as type of approximations, convergence results, rates of convergence,....
  - Theory for MDP's has reached a rather high degree of maturity, although the classical tools such as value iteration, policy iteration and linear programming, and their various extensions, are not applicable in practice. We believe that the theoretical progress of MDP's must be in parallel with the corresponding numerical developments. Therefore, solving

MDP's numerically is an awkward and important problem both from the theoretical and practical point of view. In order to meet this challenge, the fields of neural networks, neuro-dynamic programming and approximate dynamic programming became recently an active area of research. Such methods found their roots in heuristic approaches, but theoretical results for convergence results are mainly obtained in the context of finite MDP's. Hence, an ambitious challenge is to investigate such numerical problems but for models with general state and action spaces. Our motivation is to develop theoretically consistent computational approaches for approximating optimal value functions and finding optimal policies.

– An effort has been devoted to the development of efficient computational methods in the setting of communication networks. These are complex dynamical systems composed of several interacting nodes that exhibit important congestion phenomena as their level of interaction grows. The dynamics of such systems are affected by the randomness of their underlying events (e.g., arrivals of http requests to a web-server) and are described stochastically in terms of queueing network models. These are mathematical tools that allow one to predict the performance achievable by the system, to optimize the network configuration, to perform capacity-planning studies, etc. These objectives are usually difficult to achieve without a mathematical model because Internet systems are huge in size. However, because of the exponential growth of their state spaces, an exact analysis of queueing network models is generally difficult to obtain. Given this complexity, we have developed analyses in some limiting regime of practical interest (e.g., systems size grows to infinity). This approach is helpful to obtain a simpler mathematical description of the system under investigation, which leads to the direct definition of efficient, though approximate, computational methods and also allows to investigate other aspects such as Nash equilibria.

The second objective of the team is to study some theoretical aspects related to MDPs such as convex analytical methods and singular perturbation. Analysis of various problems arising in MDPs leads to a large variety of interesting mathematical problems.

MATHRISK Project-Team

3. Research Program

3.1. Dependence modeling

Participants: Aurélien Alfonsi, Benjamin Jourdain, Damien Lamberton, Bernard Lapeyre.

The volatility is a key concept in modern mathematical finance, and an indicator of the market stability. Risk management and associated instruments depend strongly on the volatility, and volatility modeling has thus become a crucial issue in the finance industry. Of particular importance is the assets *dependence* modeling. The calibration of models for a single asset can now be well managed by banks but modeling of dependence is the bottleneck to efficiently aggregate such models. A typical issue is how to go from the individual evolution of each stock belonging to an index to the joint modeling of these stocks. In this perspective, we want to model stochastic volatility in a *multidimensional* framework. To handle these questions mathematically, we have to deal with stochastic differential equations that are defined on matrices in order to model either the instantaneous covariance or the instantaneous correlation between the assets. From a numerical point of view, such models are very demanding since the main indexes include generally more than thirty assets. It is therefore necessary to develop efficient numerical methods for pricing options and calibrating such models to market data. As a first application, modeling the dependence between assets allows us to better handle derivatives products on a basket. It would give also a way to price and hedge consistenly single-asset and basket products. Besides, it can be a way to capture how the market estimates the dependence between assets. This could give some insights on how the market anticipates the systemic risk.

3.2. Liquidity risk

Participants: Aurélien Alfonsi, Agnès Sulem, Antonino Zanette.

The financial crisis has caused an increased interest in mathematical finance studies which take into account the market incompleteness issue and the liquidity risk. Loosely speaking, liquidity risk is the risk that comes from the difficulty of selling (or buying) an asset. At the extreme, this may be the impossibility to sell an asset, which occurred for “junk assets” during the subprime crisis. Hopefully, it is in general possible to sell assets, but this may have some cost. Let us be more precise. Usually, assets are quoted on a market with a Limit Order Book (LOB) that registers all the waiting limit buy and sell orders for this asset. The bid (resp. ask) price is the most expensive (resp. cheapest) waiting buy or sell order. If a trader wants to sell a single asset, he will sell it at the bid price. Instead, if he wants to sell a large quantity of assets, he will have to sell them at a lower price in order to match further waiting buy orders. This creates an extra cost, and raises important issues. From a short-term perspective (from few minutes to some days), this may be interesting to split the selling order and to focus on finding optimal selling strategies. This requires to model the market microstructure, i.e. how the market reacts in a short time-scale to execution orders. From a long-term perspective (typically, one month or more), one has to understand how this cost modifies portfolio managing strategies (especially delta-hedging or optimal investment strategies). At this time-scale, there is no need to model precisely the market microstructure, but one has to specify how the liquidity costs aggregate.

3.2.1. Long term liquidity risk.

On a long-term perspective, illiquidity can be approached via various ways: transactions costs [41], [42], [53], [61], [67], [87], [83], delay in the execution of the trading orders [88], [86], [57], trading constraints or restriction on the observation times (see e.g. [63] and references herein). As far as derivative products are concerned, one has to understand how delta-hedging strategies have to be modified. This has been considered for example by Cetin, Jarrow and Protter [85]. We plan to contribute on these various aspects of liquidity risk modeling and associated stochastic optimization problems. Let us mention here that the price impact generated by the trades of the investor is often neglected with a long-term perspective. This seems acceptable since the investor has time enough to trade slowly in order to eliminate its market impact. Instead, when the investor wants to make significant trades on a very short time horizon, it is crucial to take into account and to model how prices are modified by these trades. This question is addressed in the next paragraph on market microstructure.

3.2.2. Market microstructure.

The European directive MIFID has increased the competition between markets (NYSE-Euronext, Nasdaq, LSE and new competitors). As a consequence, the cost of posting buy or sell orders on markets has decreased, which has stimulated the growth of market makers. Market makers are posting simultaneously bid and ask orders on a same stock, and their profit comes from the bid-ask spread. Basically, their strategy is a "round-trip" (i.e. their position is unchanged between the beginning and the end of the day) that has generated a positive cash flow.

These new rules have also greatly stimulated research on market microstructure modeling. From a practitioner point of view, the main issue is to solve the so-called "optimal execution problem": given a deadline T, what is the optimal strategy to buy (or sell) a given amount of shares that achieves the minimal expected cost? For large amounts, it may be optimal to split the order into smaller ones. This is of course a crucial issue for brokers, but also market makers that are looking for the optimal round-trip.

Solving the optimal execution problem is not only an interesting mathematical challenge. It is also a mean to better understand market viability, high frequency arbitrage strategies and consequences of the competition between markets. For example when modeling the market microstructure, one would like to find conditions that allow or exclude round trips. Beyond this, even if round trips are excluded, it can happen that an optimal selling strategy is made with large intermediate buy trades, which is unlikely and may lead to market instability.

We are interested in finding synthetic market models in which we can describe and solve the optimal execution problem. A. Alfonsi and A. Schied (Mannheim University) [45] have already proposed a simple Limit Order Book model (LOB) in which an explicit solution can be found for the optimal execution problem. We are now interested in considering more sophisticated models that take into account realistic features of the market such as short memory or stochastic LOB. This is mid term objective. At a long term perspective one would like to bridge these models to the different agent behaviors, in order to understand the effect of the different quotation mechanisms (transaction costs for limit orders, tick size, etc.) on the market stability.

3.3. Contagion modeling and systemic risk

Participants: Benjamin Jourdain, Agnès Sulem.

After the recent financial crisis, systemic risk has emerged as one of the major research topics in mathematical finance. The scope is to understand and model how the bankruptcy of a bank (or a large company) may or not induce other bankruptcies. By contrast with the traditional approach in risk management, the focus is no longer on modeling the risks faced by a single financial institution, but on modeling the complex interrelations between financial institutions and the mechanisms of distress propagation among these. Ideally, one would like to be able to find capital requirements (such as the one proposed by the Basel committee) that ensure that the probability of multiple defaults is below some level.

The mathematical modeling of default contagion, by which an economic shock causing initial losses and default of a few institutions is amplified due to complex linkages, leading to large scale defaults, can be addressed by various techniques, such as network approaches (see in particular R. Cont et al. [46] and A. Minca [72]) or mean field interaction models (Garnier-Papanicolaou-Yang [62]). The recent approach in [46] seems very promising. It describes the financial network approach as a weighted directed graph, in which nodes represent financial institutions and edges the exposures between them. Distress propagation in a financial system may be modeled as an epidemics on this graph. In the case of incomplete information on the structure of the interbank network, cascade dynamics may be reduced to the evolution of a multi-dimensional Markov chain that corresponds to a sequential discovery of exposures and determines at any time the size of contagion. Little has been done so far on the *control* of such systems in order to reduce the systemic risk and we aim to contribute to this domain.

3.4. Stochastic analysis and numerical probability

3.4.1. Stochastic control

Participants: Vlad Bally, Jean-Philippe Chancelier, Marie-Claire Quenez, Agnès Sulem.

The financial crisis has caused an increased interest in mathematical finance studies which take into account the market incompleteness issue and the default risk modeling, the interplay between information and performance, the model uncertainty and the associated robustness questions, and various nonlinearities. We address these questions by further developing the theory of stochastic control in a broad sense, including stochastic optimization, nonlinear expectations, Malliavin calculus, stochastic differential games and various aspects of optimal stopping.

3.4.2. Optimal stopping

Participants: Aurélien Alfonsi, Benjamin Jourdain, Damien Lamberton, Agnès Sulem, Marie-Claire Quenez.

The theory of American option pricing has been an incite for a number of research articles about optimal stopping. Our recent contributions in this field concern optimal stopping in models with jumps, irregular obstacles, free boundary analysis, reflected BSDEs.

3.4.3. Simulation of stochastic differential equations

Participants: Benjamin Jourdain, Aurélien Alfonsi, Vlad Bally, Damien Lamberton, Bernard Lapeyre, Jérôme Lelong, Céline Labart.

Effective numerical methods are crucial in the pricing and hedging of derivative securities. The need for more complex models leads to stochastic differential equations which cannot be solved explicitly, and the development of discretization techniques is essential in the treatment of these models. The project MathRisk addresses fundamental mathematical questions as well as numerical issues in the following (non exhaustive) list of topics: Multidimensional stochastic differential equations, High order discretization schemes, Singular stochastic differential equations, Backward stochastic differential equations.

3.4.4. Monte-Carlo simulations

Participants: Benjamin Jourdain, Aurélien Alfonsi, Damien Lamberton, Vlad Bally, Bernard Lapeyre, Ahmed Kebaier, Céline Labart, Jérôme Lelong, Antonino Zanette.

Monte-Carlo methods is a very useful tool to evaluate prices especially for complex models or options. We carry on research on *adaptive variance reduction methods* and to use *Monte-Carlo methods for calibration* of advanced models.

This activity in the MathRisk team is strongly related to the development of the Premia software.

3.4.5. Malliavin calculus and applications in finance

Participants: Vlad Bally, Arturo Kohatsu-Higa, Agnès Sulem, Antonino Zanette.

The original Stochastic Calculus of Variations, now called the Malliavin calculus, was developed by Paul Malliavin in 1976 [70]. It was originally designed to study the smoothness of the densities of solutions of stochastic differential equations. One of its striking features is that it provides a probabilistic proof of the celebrated Hörmander theorem, which gives a condition for a partial differential operator to be hypoelliptic. This illustrates the power of this calculus. In the following years a lot of probabilists worked on this topic and the theory was developed further either as analysis on the Wiener space or in a white noise setting. Many applications in the field of stochastic calculus followed. Several monographs and lecture notes (for example D. Nualart [74], D. Bell [52] D. Ocone [76], B. Øksendal [89]) give expositions of the subject. See also V. Bally [47] for an introduction to Malliavin calculus.

From the beginning of the nineties, applications of the Malliavin calculus in finance have appeared : In 1991 Karatzas and Ocone showed how the Malliavin calculus, as further developed by Ocone and others, could be used in the computation of hedging portfolios in complete markets [75].

Since then, the Malliavin calculus has raised increasing interest and subsequently many other applications to finance have been found [71], such as minimal variance hedging and Monte Carlo methods for option pricing. More recently, the Malliavin calculus has also become a useful tool for studying insider trading models and some extended market models driven by Lévy processes or fractional Brownian motion.

We give below an idea why Malliavin calculus may be a useful instrument for probabilistic numerical methods.

We recall that the theory is based on an integration by parts formula of the form $E(f'(X)) = E(f(X)Q)$. Here X is a random variable which is supposed to be "smooth" in a certain sense and non-degenerated. A basic example is to take $X = \sigma\Delta$ where Δ is a standard normally distributed random variable and σ is a strictly positive number. Note that an integration by parts formula may be obtained just by using the usual integration by parts in the presence of the Gaussian density. But we may go further and take X to be an aggregate of Gaussian random variables (think for example of the Euler scheme for a diffusion process) or the limit of such simple functionals.

An important feature is that one has a relatively explicit expression for the weight Q which appears in the integration by parts formula, and this expression is given in terms of some Malliavin-derivative operators.

Let us now look at one of the main consequences of the integration by parts formula. If one considers the *Dirac* function $\delta_x(y)$, then $\delta_x(y) = H'(y-x)$ where H is the *Heaviside* function and the above integration by parts formula reads $E(\delta_x(X)) = E(H(X-x)Q)$, where $E(\delta_x(X))$ can be interpreted as the density of the random variable X. We thus obtain an integral representation of the density of the law of X. This is the starting point of the approach to the density of the law of a diffusion process: the above integral representation allows us to prove that under appropriate hypothesis the density of X is smooth and also to derive upper and lower bounds for it. Concerning simulation by Monte Carlo methods, suppose that you want to compute $E(\delta_x(y)) \sim \frac{1}{M}\sum_{i=1}^{M}\delta_x(X^i)$ where $X^1,...,X^M$ is a sample of X. As X has a law which is absolutely continuous with respect to the Lebesgue measure, this will fail because no X^i hits exactly x. But if you are able to simulate the weight Q as well (and this is the case in many applications because of the explicit form mentioned above) then you may try to compute $E(\delta_x(X)) = E(H(X-x)Q) \sim \frac{1}{M}\sum_{i=1}^{M}E(H(X^i-x)Q^i)$. This basic remark formula leads to efficient methods to compute by a Monte Carlo method some irregular quantities as derivatives of option prices with respect to some parameters (the *Greeks*) or conditional expectations, which appear in the pricing of American options by the dynamic programming). See the papers by Fournié et al [60] and [59] and the papers by Bally et al., Benhamou, Bermin et al., Bernis et al., Cvitanic et al., Talay and Zheng and Temam in [69].

L. Caramellino, A. Zanette and V. Bally have been concerned with the computation of conditional expectations using Integration by Parts formulas and applications to the numerical computation of the price and the Greeks (sensitivities) of American or Bermudean options. The aim of this research was to extend a paper of Reigner and Lions who treated the problem in dimension one to higher dimension - which represent the real challenge in this field. Significant results have been obtained up to dimension 5 [51] and the corresponding algorithms have been implemented in the Premia software.

Moreover, there is an increasing interest in considering jump components in the financial models, especially motivated by calibration reasons. Algorithms based on the integration by parts formulas have been developed in order to compute Greeks for options with discontinuous payoff (e.g. digital options). Several papers and two theses (M. Messaoud and M. Bavouzet defended in 2006) have been published on this topic and the corresponding algorithms have been implemented in Premia. Malliavin Calculus for jump type diffusions - and more general for random variables with locally smooth law - represents a large field of research, also for applications to credit risk problems.

The Malliavin calculus is also used in models of insider trading. The "enlargement of filtration" technique plays an important role in the modeling of such problems and the Malliavin calculus can be used to obtain general results about when and how such filtration enlargement is possible. See the paper by P. Imkeller in [69]). Moreover, in the case when the additional information of the insider is generated by adding the information about the value of one extra random variable, the Malliavin calculus can be used to find explicitly the optimal portfolio of an insider for a utility optimization problem with logarithmic utility. See the paper by J.A. León, R. Navarro and D. Nualart in [69]).

A. Kohatsu Higa and A. Sulem have studied a controlled stochastic system whose state is described by a stochastic differential equation with anticipating coefficients. These SDEs can be interpreted in the sense of *forward integrals*, which are the natural generalization of the semimartingale integrals, as introduced by Russo and Valois [82]. This methodology has been applied for utility maximization with insiders.

REGULARITY Project-Team

3. Research Program

3.1. Theoretical aspects: probabilistic modeling of irregularity

The modeling of essentially irregular phenomena is an important challenge, with an emphasis on understanding the sources and functions of this irregularity. Probabilistic tools are well-adapted to this task, provided one can design stochastic models for which the regularity can be measured and controlled precisely. Two points deserve special attention:

- first, the study of regularity has to be *local*. Indeed, in most applications, one will want to act on a system based on local temporal or spatial information. For instance, detection of arrhythmias in ECG or of krachs in financial markets should be performed in "real time", or, even better, ahead of time. In this sense, regularity is a *local* indicator of the *local* health of a system.
- Second, although we have used the term "irregularity" in a generic and somewhat vague sense, it seems obvious that, in real-world phenomena, regularity comes in many colors, and a rigorous analysis should distinguish between them. As an example, at least two kinds of irregularities are present in financial logs: the local "roughness" of the records, and the local density and height of jumps. These correspond to two different concepts of regularity (in technical terms, Hölder exponents and local index of stability), and they both contribute a different manner to financial risk.

In view of the above, the *Regularity* team focuses on the design of methods that:

1. define and study precisely various relevant measures of local regularity,
2. allow to build stochastic models versatile enough to mimic the rapid variations of the different kinds of regularities observed in real phenomena,
3. allow to estimate as precisely and rapidly as possible these regularities, so as to alert systems in charge of control.

Our aim is to address the three items above through the design of mathematical tools in the field of probability (and, to a lesser extent, statistics), and to apply these tools to uncertainty management as described in the following section. We note here that we do not intend to address the problem of controlling the phenomena based on regularity, that would naturally constitute an item 4 in the list above. Indeed, while we strongly believe that generic tools may be designed to measure and model regularity, and that these tools may be used to analyze real-world applications, in particular in the field of uncertainty management, it is clear that, when it comes to control, application-specific tools are required, that we do not wish to address.

The research topics of the *Regularity* team can be roughly divided into two strongly interacting axes, corresponding to two complementary ways of studying regularity:

1. developments of tools allowing to characterize, measure and estimate various notions of local regularity, with a particular emphasis on the stochastic frame,
2. definition and fine analysis of stochastic models for which some aspects of local regularity may be prescribed.

These two aspects are detailed in sections 3.2 and 3.3 below.

3.2. Tools for characterizing and measuring regularity

Fractional Dimensions

Although the main focus of our team is on characterizing *local* regularity, on occasions, it is interesting to use a *global* index of regularity. Fractional dimensions provide such an index. In particular, the *regularization dimension*, that was defined in [31], is well adapted to the study stochastic processes, as its definition allows to build robust estimators in an easy way. Since its introduction, regularization dimension has been used by various teams worldwide in many different applications including the characterization of certain stochastic processes, statistical estimation, the study of mammographies or galactograms for breast carcinomas detection, ECG analysis for the study of ventricular arrhythmia, encephalitis diagnosis from EEG, human skin analysis, discrimination between the nature of radioactive contaminations, analysis of porous media textures, well-logs data analysis, agro-alimentary image analysis, road profile analysis, remote sensing, mechanical systems assessment, analysis of video games, ...(see http://regularity.saclay.inria.fr/theory/localregularity/biblioregdim for a list of works using the regularization dimension).

Hölder exponents

The simplest and most popular measures of local regularity are the pointwise and local Hölder exponents. For a stochastic process $\{X(t)\}_{t\in\mathbb{R}}$ whose trajectories are continuous and nowhere differentiable, these are defined, at a point t_0, as the random variables:

$$\alpha_X(t_0,\omega)=\sup\left\{\alpha:\limsup_{\rho\to 0}\sup_{t,u\in B(t_0,\rho)}\frac{|X_t-X_u|}{\rho^\alpha}<\infty\right\}, \tag{63}$$

and

$$\widetilde{\alpha}_X(t_0,\omega)=\sup\left\{\alpha:\limsup_{\rho\to 0}\sup_{t,u\in B(t_0,\rho)}\frac{|X_t-X_u|}{\|t-u\|^\alpha}<\infty\right\}. \tag{64}$$

Although these quantities are in general random, we will omit as is customary the dependency in ω and X and write $\alpha(t_0)$ and $\widetilde{\alpha}(t_0)$ instead of $\alpha_X(t_0,\omega)$ and $\widetilde{\alpha}_X(t_0,\omega)$.

The random functions $t\mapsto\alpha_X(t_0,\omega)$ and $t\mapsto\widetilde{\alpha}_X(t_0,\omega)$ are called respectively the pointwise and local Hölder functions of the process X.

The pointwise Hölder exponent is a very versatile tool, in the sense that the set of pointwise Hölder functions of continuous functions is quite large (it coincides with the set of lower limits of sequences of continuous functions [6]). In this sense, the pointwise exponent is often a more precise tool (*i.e.* it varies in a more rapid way) than the local one, since local Hölder functions are always lower semi-continuous. This is why, in particular, it is the exponent that is used as a basis ingredient in multifractal analysis (see section 3.2). For certain classes of stochastic processes, and most notably Gaussian processes, it has the remarkable property that, at each point, it assumes an almost sure value [18]. SRP, mBm, and processes of this kind (see sections 3.3 and 3.3) rely on the sole use of the pointwise Hölder exponent for prescribing the regularity.

However, α_X obviously does not give a complete description of local regularity, even for continuous processes. It is for instance insensitive to “oscillations”, contrarily to the local exponent. A simple example in the deterministic frame is provided by the function $x^\gamma\sin(x^{-\beta})$, where γ,β are positive real numbers. This so-called “chirp function” exhibits two kinds of irregularities: the first one, due to the term x^γ is measured by the pointwise Hölder exponent. Indeed, $\alpha(0)=\gamma$. The second one is due to the wild oscillations around 0, to which α is blind. In contrast, the local Hölder exponent at 0 is equal to $\frac{\gamma}{1+\beta}$, and is thus influenced by the oscillatory behaviour.

Another, related, drawback of the pointwise exponent is that it is not stable under integro-differentiation, which sometimes makes its use complicated in applications. Again, the local exponent provides here a useful complement to α, since $\widetilde{\alpha}$ is stable under integro-differentiation.

Both exponents have proved useful in various applications, ranging from image denoising and segmentation to TCP traffic characterization. Applications require precise estimation of these exponents.

Stochastic 2-microlocal analysis

Neither the pointwise nor the local exponents give a complete characterization of the local regularity, and, although their joint use somewhat improves the situation, it is far from yielding the complete picture.

A fuller description of local regularity is provided by the so-called *2-microlocal analysis*, introduced by J.M. Bony [46]. In this frame, regularity at each point is now specified by two indices, which makes the analysis and estimation tasks more difficult. More precisely, a function f is said to belong to the *2-microlocal space*$C_{x_0}^{s,s'}$, where $s+s'>0, s'<0$, if and only if its $m=[s+s']-$th order derivative exists around x_0, and if there exists $\delta>0$, a polynomial P with degree lower than $[s]-m$, and a constant C, such that

$$\left|\frac{\partial^m f(x)-P(x)}{|x-x_0|^{[s]-m}}-\frac{\partial^m f(y)-P(y)}{|y-x_0|^{[s]-m}}\right|\leq C|x-y|^{s+s'-m}(|x-y|+|x-x_0|)^{-s'-[s]+m}$$

for all x,y such that $0<|x-x_0|<\delta$, $0<|y-x_0|<\delta$. This characterization was obtained in [25], [32]. See [53], [54] for other characterizations and results. These spaces are stable through integro-differentiation, i.e. $f\in C_x^{s,s'}$ if and only if $f'\in C_x^{s-1,s'}$. Knowing to which space f belongs thus allows to predict the evolution of its regularity after derivation, a useful feature if one uses models based on some kind differential equations. A lot of work remains to be done in this area, in order to obtain more general characterizations, to develop robust estimation methods, and to extend the "2-microlocal formalism" : this is a tool allowing to detect which space a function belongs to, from the computation of the Legendre transform of an auxiliary function known as its *2-microlocal spectrum*. This spectrum provide a wealth of information on the local regularity.

In [18], we have laid some foundations for a stochastic version of 2-microlocal analysis. We believe this will provide a fine analysis of the local regularity of random processes in a direction different from the one detailed for instance in [55].We have defined random versions of the 2-microlocal spaces, and given almost sure conditions for continuous processes to belong to such spaces. More precise results have also been obtained for Gaussian processes. A preliminary investigation of the 2-microlocal behaviour of Wiener integrals has been performed.

Multifractal analysis of stochastic processes

A direct use of the local regularity is often fruitful in applications. This is for instance the case in RR analysis or terrain modeling. However, in some situations, it is interesting to supplement or replace it by a more global approach known as *multifractal analysis* (MA). The idea behind MA is to group together all points with same regularity (as measured by the pointwise Hölder exponent) and to measure the "size" of the sets thus obtained [28], [47], [50]. There are mainly two ways to do so, a geometrical and a statistical one.

In the geometrical approach, one defines the *Hausdorff multifractal spectrum* of a process or function X as the function: $\alpha\mapsto f_h(\alpha)=\dim\{t:\alpha_X(t)=\alpha\}$, where $\dim E$ denotes the Hausdorff dimension of the set E. This gives a fine measure-theoretic information, but is often difficult to compute theoretically, and almost impossible to estimate on numerical data.

The statistical path to MA is based on the so-called *large deviation multifractal spectrum*:

$$f_g(\alpha)=\lim_{\varepsilon\to 0}\liminf_{n\to\infty}\frac{\log\ N_n^\varepsilon(\alpha)}{\log\ n},$$

where:

$$N_n^\varepsilon(\alpha)=\#\{k:\alpha-\varepsilon\leq\alpha_n^k\leq\alpha+\varepsilon\},$$

and α_n^k is the "coarse grained exponent" corresponding to the interval $I_n^k=\left[\frac{k}{n},\frac{k+1}{n}\right]$, *i.e.*:

$$\alpha_n^k=\frac{\log|Y_n^k|}{-\log\ n}.$$

Here, Y_n^k is some quantity that measures the variation of X in the interval I_n^k, such as the increment, the oscillation or a wavelet coefficient.

The large deviation spectrum is typically easier to compute and to estimate than the Hausdorff one. In addition, it often gives more relevant information in applications.

Under very mild conditions (*e.g.* for instance, if the support of f_g is bounded, [27]) the concave envelope of f_g can be computed easily from an auxiliary function, called the *Legendre multifractal spectrum*. To do so, one basically interprets the spectrum f_g as a rate function in a large deviation principle (LDP): define, for $q \in \mathbb{R}$,

$$S_n(q) = \sum_{k=0}^{n-1} |Y_n^k|^q, \tag{65}$$

with the convention $0^q := 0$ for all $q \in \mathbb{R}$. Let:

$$\tau(q) = \liminf_{n\to\infty} \frac{\log S_n(q)}{-\log(n)}.$$

The Legendre multifractal spectrum of X is defined as the Legendre transform τ^* of τ:

$$f_l(\alpha) := \tau^*(\alpha) := \inf_{q\in\mathbb{R}} (q\alpha - \tau(q)).$$

To see the relation between f_g and f_l, define the sequence of random variables $Z_n := \log |Y_n^k|$ where the randomness is through a choice of k uniformly in $\{0, ..., n-1\}$. Consider the corresponding moment generating functions:

$$c_n(q) := -\frac{\log E_n[\exp{(qZ_n)}]}{\log(n)}$$

where E_n denotes expectation with respect to P_n, the uniform distribution on $\{0, ..., n-1\}$. A version of Gärtner-Ellis theorem ensures that if $\lim c_n(q)$ exists (in which case it equals $1 + \tau(q)$), and is differentiable, then $c^* = f_g - 1$. In this case, one says that the *weak multifractal formalism* holds, *i.e.* $f_g = f_l$. In favorable cases, this also coincides with f_h, a situation referred to as the *strong multifractal formalism*.

Multifractal spectra subsume a lot of information about the distribution of the regularity, that has proved useful in various situations. A most notable example is the strong correlation reported recently in several works between the narrowing of the multifractal spectrum of ECG and certain pathologies of the heart [51], [52]. Let us also mention the multifractality of TCP traffic, that has been both observed experimentally and proved on simplified models of TCP [2], [44].

Another colour in local regularity: jumps

As noted above, apart from Hölder exponents and their generalizations, at least another type of irregularity may sometimes be observed on certain real phenomena: discontinuities, which occur for instance on financial logs and certain biomedical signals. In this frame, it is of interest to supplement Hölder exponents and their extensions with (at least) an additional index that measures the local intensity and size of jumps. This is a topic we intend to pursue in full generality in the near future. So far, we have developed an approach in the particular frame of *multistable processes*. We refer to section 3.3 for more details.

3.3. Stochastic models

The second axis in the theoretical developments of the *Regularity* team aims at defining and studying stochastic processes for which various aspects of the local regularity may be prescribed.

Multifractional Brownian motion

One of the simplest stochastic process for which some kind of control over the Hölder exponents is possible is probably fractional Brownian motion (fBm). This process was defined by Kolmogorov and further studied by Mandelbrot and Van Ness, followed by many authors. The so-called “moving average” definition of fBm reads as follows:

$$Y_t = \int_{-\infty}^{0} \left[(t-u)^{H-\frac{1}{2}} - (-u)^{H-\frac{1}{2}} \right] .\mathbb{W}(du) + \int_0^t (t-u)^{H-\frac{1}{2}} .\mathbb{W}(du),$$

where $\mathbb{W}$ denotes the real white noise. The parameter H ranges in $(0,1)$, and it governs the pointwise regularity: indeed, almost surely, at each point, both the local and pointwise Hölder exponents are equal to H.

Although varying H yields processes with different regularity, the fact that the exponents are constant along any single path is often a major drawback for the modeling of real world phenomena. For instance, fBm has often been used for the synthesis natural terrains. This is not satisfactory since it yields images lacking crucial features of real mountains, where some parts are smoother than others, due, for instance, to erosion.

It is possible to generalize fBm to obtain a Gaussian process for which the pointwise Hölder exponent may be tuned at each point: the *multifractional Brownian motion (mBm)* is such an extension, obtained by substituting the constant parameter $H \in (0,1)$ with a *regularity function*$H : \mathbb{R}_+ \to (0,1)$.

mBm was introduced independently by two groups of authors: on the one hand, Peltier and Levy-Vehel [29] defined the mBm $\{X_t;\ t \in \mathbb{R}_+\}$ from the moving average definition of the fractional Brownian motion, and set:

$$X_t = \int_{-\infty}^{0} \left[(t-u)^{H(t)-\frac{1}{2}} - (-u)^{H(t)-\frac{1}{2}} \right] .\mathbb{W}(du) + \int_0^t (t-u)^{H(t)-\frac{1}{2}} .\mathbb{W}(du),$$

On the other hand, Benassi, Jaffard and Roux [45] defined the mBm from the harmonizable representation of the fBm, *i.e.*:

$$X_t = \int_{\mathbb{R}} \frac{e^{it\xi} - 1}{|\xi|^{H(t)+\frac{1}{2}}} .\widehat{\mathbb{W}}(d\xi),$$

where $\widehat{\mathbb{W}}$ denotes the complex white noise.

The Hölder exponents of the mBm are prescribed almost surely: the pointwise Hölder exponent is $\alpha_X(t) = H(t) \wedge \alpha_H(t)$ a.s., and the local Hölder exponent is $\widetilde{\alpha}_X(t) = H(t) \wedge \widetilde{\alpha}_H(t)$ a.s. Consequently, the regularity of the sample paths of the mBm are determined by the function H or by its regularity. The multifractional Brownian motion is our prime example of a stochastic process with prescribed local regularity.

The fact that the local regularity of mBm may be tuned *via* a functional parameter has made it a useful model in various areas such as finance, biomedicine, geophysics, image analysis, ... A large number of studies have been devoted worldwide to its mathematical properties, including in particular its local time. In addition, there is now a rather strong body of work dealing the estimation of its functional parameter, *i.e.* its local regularity. See http://regularity.saclay.inria.fr/theory/stochasticmodels/bibliombm for a partial list of works, applied or theoretical, that deal with mBm.

Self-regulating processes

We have recently introduced another class of stochastic models, inspired by mBm, but where the local regularity, instead of being tuned "exogenously", is a function of the amplitude. In other words, at each point t, the Hölder exponent of the process X verifies almost surely $\alpha_X(t) = g(X(t))$, where g is a fixed deterministic function verifying certain conditions. A process satisfying such an equation is generically termed a *self-regulating process* (SRP). The particular process obtained by adapting adequately mBm is called the self-regulating multifractional process [3]. Another instance is given by modifying the Lévy construction of Brownian motion [4]. The motivation for introducing self-regulating processes is based on the following general fact: in nature, the local regularity of a phenomenon is often related to its amplitude. An intuitive example is provided by natural terrains: in young mountains, regions at higher altitudes are typically more irregular than regions at lower altitudes. We have verified this fact experimentally on several digital elevation models [8]. Other natural phenomena displaying a relation between amplitude and exponent include temperatures records and RR intervals extracted from ECG [9].

To build the SRMP, one starts from a field of fractional Brownian motions $B(t, H)$, where (t, H) span $[0, 1] \times [a, b]$ and $0 < a < b < 1$. For each fixed H, $B(t, H)$ is a fractional Brownian motion with exponent H. Denote:

$$\underline{\overline{X}}_{\alpha'}^{\beta'} = \alpha' + (\beta' - \alpha') \frac{X - \min_K(X)}{\max_K(X) - \min_K(X)}$$

the affine rescaling between α' and β' of an arbitrary continuous random field over a compact set K. One considers the following (stochastic) operator, defined almost surely:

$$\begin{array}{rcl} \Lambda_{\alpha',\beta'} : \mathcal{C}([0,1],[\alpha,\beta]) & \to & \mathcal{C}([0,1],[\alpha,\beta]) \\ Z(.) & \mapsto & \underline{\overline{B(., g(Z(.))}}_{\alpha'}^{\beta'} \end{array}$$

where $\alpha \le \alpha' < \beta' \le \beta$, α and β are two real numbers, and α', β' are random variables adequately chosen. One may show that this operator is contractive with respect to the sup-norm. Its unique fixed point is the SRMP. Additional arguments allow to prove that, indeed, the Hölder exponent at each point is almost surely $g(t)$.

An example of a two dimensional SRMP with function $g(x) = 1 - x^2$ is displayed on figure 1 .

We believe that SRP open a whole new and very promising area of research.

Multistable processes

Non-continuous phenomena are commonly encountered in real-world applications, *e.g.* financial records or EEG traces. For such processes, the information brought by the Hölder exponent must be supplemented by some measure of the density and size of jumps. Stochastic processes with jumps, and in particular Lévy processes, are currently an active area of research.

The simplest class of non-continuous Lévy processes is maybe the one of stable processes [56]. These are mainly characterized by a parameter $\alpha \in (0, 2]$, the *stability index* ($\alpha = 2$ corresponds to the Gaussian case, that we do not consider here). This index measures in some precise sense the intensity of jumps. Paths of stable processes with α close to 2 tend to display "small jumps", while, when α is near 0, their aspect is governed by large ones.

In line with our quest for the characterization and modeling of various notions of local regularity, we have defined *multistable processes*. These are processes which are "locally" stable, but where the stability index α is now a function of time. This allows to model phenomena which, at times, are "almost continuous", and at others display large discontinuities. Such a behaviour is for instance obvious on almost any sufficiently long financial record.

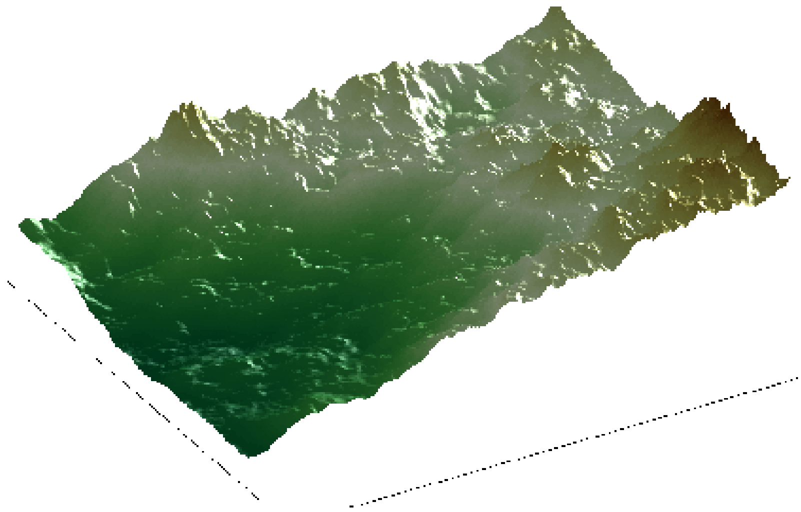


Figure 1. Self-regulating miltifractional process with $g(x) = 1 - x^2$

More formally, a multistable process is a process which is, at each time u, tangent to a stable process [49]. Recall that a process Y is said to be tangent at u to the process Y'_u if:

$$\lim_{r \to 0} \frac{Y(u+rt) - Y(u)}{r^h} = Y'_u(t), \tag{66}$$

where the limit is understood either in finite dimensional distributions or in the stronger sense of distributions. Note Y'_u may and in general will vary with u.

One approach to defining multistable processes is similar to the one developed for constructing mBm [29]: we consider fields of stochastic processes $X(t,u)$, where t is time and u is an independent parameter that controls the variation of α. We then consider a "diagonal" process $Y(t) = X(t,t)$, which will be, under certain conditions, "tangent" at each point t to a process $t \mapsto X(t,u)$.

A particular class of multistable processes, termed "linear multistable multifractional motions" (lmmm) takes the following form [11], [10]. Let $(E, \mathcal{E}, m)$ be a σ-finite measure space, and Π be a Poisson process on $E \times \mathbb{R}$ with mean measure $m \times \mathcal{L}$ ($\mathcal{L}$ denotes the Lebesgue measure). An lmmm is defined as:

$$Y(t) = a(t) \sum_{(\mathsf{X},\mathsf{Y}) \in \Pi} \mathsf{Y}^{<-1/\alpha(t)>} \left(|t - \mathsf{X}|^{h(t)-1/\alpha(t)} - |\mathsf{X}|^{h(t)-1/\alpha(t)} \right) \quad (t \in \mathbb{R}). \tag{67}$$

where $x^{<y>} := \text{sign}(x)|x|^y$, $a : \mathbb{R} \to \mathbb{R}^+$ is a C^1 function and $\alpha : \mathbb{R} \to (0,2)$ and $h : \mathbb{R} \to (0,1)$ are C^2 functions.

In fact, lmmm are somewhat more general than said above: indeed, the couple (h, α) allows to prescribe at each point, under certain conditions, both the pointwise Hölder exponent and the local intensity of jumps. In this sense, they generalize both the mBm and the linear multifractional stable motion [57]. From a broader perspective, such multistable multifractional processes are expected to provide relevant models for TCP traces, financial logs, EEG and other phenomena displaying time-varying regularity both in terms of Hölder exponents and discontinuity structure.

Figure 2 displays a graph of an lmmm with linearly increasing α and linearly decreasing H. One sees that the path has large jumps at the beginning, and almost no jumps at the end. Conversely, it is smooth (between jumps) at the beginning, but becomes jaggier and jaggier as time evolves.

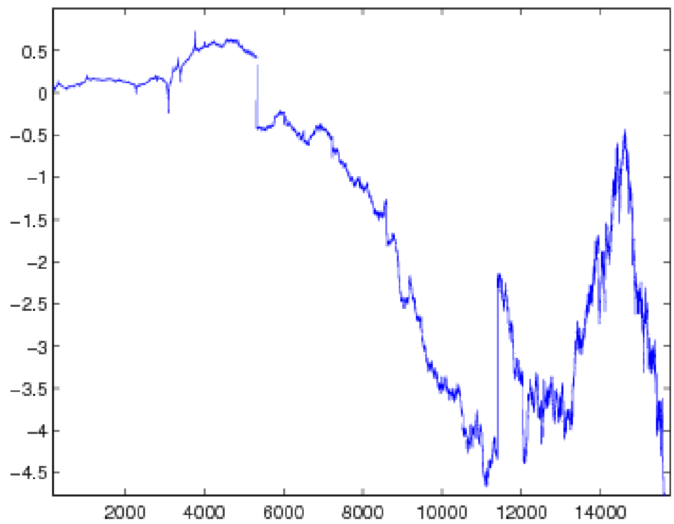


Figure 2. Linear multistable multifractional motion with linearly increasing α and linearly decreasing H

TOSCA Project-Team

3. Research Program

3.1. Research Program

Most often physicists, economists, biologists, 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. Then 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, 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.