RESEARCH CENTER

FIELD
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ACUMES Project-Team

3. Research Program

3.1. Research directions

The project develops along the following two axes:

- modeling complex systems through novel (unconventional) PDE systems, accounting for multi-scale phenomena and uncertainty;
- optimization and optimal control algorithms for systems governed by the above PDE systems.

These themes are motivated by the specific problems treated in the applications, and represent important and up-to-date issues in engineering sciences. For example, improving the design of transportation means and civil buildings, and the control of traffic flows, would result not only in better performances of the object of the optimization strategy (vehicles, buildings or road networks level of service), but also in enhanced safety and lower energy consumption, contributing to reduce costs and pollutant emissions.

3.1.1. PDE models accounting for multi-scale phenomena and uncertainties

Dynamical models consisting of evolutionary PDEs, mainly of hyperbolic type, appear classically in the applications studied by the previous Project-Team Opale (compressible flows, traffic, cell-dynamics, medicine, etc). Yet, the classical purely macroscopic approach is not able to account for some particular phenomena related to specific interactions occurring at smaller scales. These phenomena can be of greater importance when dealing with particular applications, where the "first order" approximation given by the purely macroscopic approach reveals to be inadequate. We refer for example to self-organizing phenomena observed in pedestrian flows [115], or to the dynamics of turbulent flows for which large scale / small scale vortical structures interfere [143].

Nevertheless, macroscopic models offer well known advantages, namely a sound analytical framework, fast numerical schemes, the presence of a low number of parameters to be calibrated, and efficient optimization procedures. Therefore, we are convinced of the interest of keeping this point of view as dominant, while completing the models with information on the dynamics at the small scale / microscopic level. This can be achieved through several techniques, like hybrid models, homogenization, mean field games. In this project, we will focus on the aspects detailed below.

The development of adapted and efficient numerical schemes is a mandatory completion, and sometimes ingredient, of all the approaches listed below. The numerical schemes developed by the team are based on finite volumes or finite elements techniques, and constitute an important tool in the study of the considered models, providing a necessary step towards the design and implementation of the corresponding optimization algorithms, see Section 3.1.2 .

3.1.1.1. Micro-macro couplings

Modeling of complex problems with a dominant macroscopic point of view often requires couplings with small scale descriptions. Accounting for systems heterogeneity or different degrees of accuracy usually leads to coupled PDE-ODE systems.

In the case of heterogeneous problems the coupling is "intrinsic", i.e. the two models evolve together and mutually affect each-other. For example, accounting for the impact of a large and slow vehicle (like a bus or a truck) on traffic flow leads to a strongly coupled system consisting of a (system of) conservation law(s) coupled with an ODE describing the bus trajectory, which acts as a moving bottleneck.The coupling is realized through a local unilateral moving constraint on the flow at the bus location, see [84] for an existence result and [68], [83] for numerical schemes.

If the coupling is intended to offer higher degree of accuracy at some locations, a macroscopic and a microscopic model are connected through an artificial boundary, and exchange information across it through suitable boundary conditions. See [74], [103] for some applications in traffic flow modelling, and [94], [99], [101] for applications to cell dynamics.

The corresponding numerical schemes are usually based on classical finite volume or finite element methods for the PDE, and Euler or Runge-Kutta schemes for the ODE, coupled in order to take into account the interaction fronts. In particular, the dynamics of the coupling boundaries require an accurate handling capturing the possible presence of non-classical shocks and preventing diffusion, which could produce wrong solutions, see for example [68], [83].

We plan to pursue our activity in this framework, also extending the above mentioned approaches to problems in two or higher space dimensions, to cover applications to crowd dynamics or fluid-structure interaction.

3.1.1.2. Micro-macro limits

Rigorous derivation of macroscopic models from microscopic ones offers a sound basis for the proposed modeling approach, and can provide alternative numerical schemes, see for example [75], [86] for the derivation of Lighthill-Whitham-Richards [126], [142] traffic flow model from Follow-the-Leader and [95] for results on crowd motion models (see also [117]). To tackle this aspect, we will rely mainly on two (interconnected) concepts: measure-valued solutions and mean-field limits.

The notion of **measure-valued solutions** for conservation laws was first introduced by DiPerna [87], and extensively used since then to prove convergence of approximate solutions and deduce existence results, see for example [96] and references therein. Measure-valued functions have been recently advocated as the appropriate notion of solution to tackle problems for which analytical results (such as existence and uniqueness of weak solutions in distributional sense) and numerical convergence are missing [57], [98]. We refer, for example, to the notion of solution for non-hyperbolic systems [105], for which no general theoretical result is available at present, and to the convergence of finite volume schemes for systems of hyperbolic conservation laws in several space dimensions, see [98].

In this framework, we plan to investigate and make use of measure-based PDE models for vehicular and pedestrian traffic flows. Indeed, a modeling approach based on (multi-scale) time-evolving measures (expressing the agents probability distribution in space) has been recently introduced (see the monograph [79]), and proved to be successful for studying emerging self-organised flow patterns [78]. The theoretical measure framework proves to be also relevant in addressing micro-macro limiting procedures of mean field type [106], where one lets the number of agents going to infinity, while keeping the total mass constant. In this case, one must prove that the *empirical measure*, corresponding to the sum of Dirac measures concentrated at the agents positions, converges to a measure-valued solution of the corresponding macroscopic evolution equation. We recall that a key ingredient in this approach is the use of the *Wasserstein distances* [151], [152]. Indeed, as observed in [135], the usual L^1 spaces are not natural in this context, since they don't guarantee uniqueness of solutions.

This procedure can potentially be extended to more complex configurations, like for example road networks or different classes of interacting agents, or to other application domains, like cell-dynamics.

Another powerful tool we shall consider to deal with micro-macro limits is the so-called **Mean Field Games (MFG)** technique (see the seminal paper [125]). This approach has been recently applied to some of the systems studied by the team, such as traffic flow and cell dynamics. In the context of crowd dynamics, including the case of several populations with different targets, the mean field game approach has been adopted in [64], [65], [88], [124], under the assumption that the individual behavior evolves according to a stochastic process, which gives rise to parabolic equations greatly simplifying the analysis of the system. Besides, a deterministic context is studied in [138], which considers a non-local velocity field. For cell dynamics, in order to take into account the fast processes that occur in the migration-related machinery, a framework such the one developed in [82] to handle games "where agents evolve their strategies according to the best-reply scheme on a much faster time scale than their social configuration variables" may turn out to be suitable. An alternative framework to MFG is also considered. This framework is based on the formulation of -Nash- games

constrained by the **Fokker-Planck** (FP, [53]) partial differential equations that govern the time evolution of the probability density functions -PDF- of stochastic systems and on objectives that may require to follow a given PDF trajectory or to minimize an expectation functional.

3.1.1.3. Non-local flows

Non-local interactions can be described through macroscopic models based on integro-differential equations. Systems of the type

$$\partial_t u + \mathrm{div}_{\mathbf{x}} F(t, \mathbf{x}, u, W) = 0, \qquad t > 0,\ \mathbf{x} \in \mathbb{R}^d,\ d \geq 1, \tag{1}$$

where $u = u(t, \mathbf{x}) \in \mathbb{R}^N$, $N \geq 1$ is the vector of conserved quantities and the variable $W = W(t, x, u)$ depends on an integral evaluation of u, arise in a variety of physical applications. Space-integral terms are considered for example in models for granular flows [50], sedimentation [59], supply chains [109], conveyor belts [110], biological applications like structured populations dynamics [134], or more general problems like gradient constrained equations [51]. Also, non-local in time terms arise in conservation laws with memory, starting from [81]. In particular, equations with non-local flux have been recently introduced in traffic flow modeling to account for the reaction of drivers or pedestrians to the surrounding density of other individuals, see [60], [67], [71], [107], [146]. While pedestrians are likely to react to the presence of people all around them, drivers will mainly adapt their velocity to the downstream traffic, assigning a greater importance to closer vehicles. In particular, and in contrast to classical (without integral terms) macroscopic equations, these models are able to display finite acceleration of vehicles through Lipschitz bounds on the mean velocity [60], [107] and lane formation in crossing pedestrian flows.

General analytical results on non-local conservation laws, proving existence and eventually uniqueness of solutions of the Cauchy problem for (1), can be found in [52] for scalar equations in one space dimension ($N = d = 1$), in [72] for scalar equations in several space dimensions ($N = 1$, $d \geq 1$) and in [46], [73], [77] for multi-dimensional systems of conservation laws. Besides, specific finite volume numerical methods have been developed recently in [46], [107] and [123].

Relying on these encouraging results, we aim to push a step further the analytical and numerical study of non-local models of type (1), in particular concerning well-posedness of initial - regularity of solutions, boundary value problems and high-order numerical schemes.

3.1.1.4. Uncertainty in parameters and initial-boundary data

Different sources of uncertainty can be identified in PDE models, related to the fact that the problem of interest is not perfectly known. At first, initial and boundary condition values can be uncertain. For instance, in traffic flows, the time-dependent value of inlet and outlet fluxes, as well as the initial distribution of vehicles density, are not perfectly determined [66]. In aerodynamics, inflow conditions like velocity modulus and direction, are subject to fluctuations [113], [133]. For some engineering problems, the geometry of the boundary can also be uncertain, due to structural deformation, mechanical wear or disregard of some details [90]. Another source of uncertainty is related to the value of some parameters in the PDE models. This is typically the case of parameters in turbulence models in fluid mechanics, which have been calibrated according to some reference flows but are not universal [144], [150], or in traffic flow models, which may depend on the type of road, weather conditions, or even the country of interest (due to differences in driving rules and conductors behaviour). This leads to equations with flux functions depending on random parameters [145], [148], for which the mean and the variance of the solutions can be computed using different techniques. Indeed, uncertainty quantification for systems governed by PDEs has become a very active research topic in the last years. Most approaches are embedded in a probabilistic framework and aim at quantifying statistical moments of the PDE solutions, under the assumption that the characteristics of uncertain parameters are known. Note that classical Monte-Carlo approaches exhibit low convergence rate and consequently accurate simulations require huge computational times. In this respect, some enhanced algorithms have been proposed, for example in the balance law framework [131]. Different approaches propose to modify the PDE solvers to account for this probabilistic context, for instance by defining the non-deterministic part of the solution on an orthogonal

basis (Polynomial Chaos decomposition) and using a Galerkin projection [113], [122], [127], [154] or an entropy closure method [85], or by discretizing the probability space and extending the numerical schemes to the stochastic components [45]. Alternatively, some other approaches maintain a fully deterministic PDE resolution, but approximate the solution in the vicinity of the reference parameter values by Taylor series expansions based on first- or second-order sensitivities [139], [150], [153].

Our objective regarding this topic is twofold. In a pure modeling perspective, we aim at including uncertainty quantification in models calibration and validation for predictive use. In this case, the choice of the techniques will depend on the specific problem considered [58]. Besides, we plan to extend previous works on sensitivity analysis [90], [128] to more complex and more demanding problems. In particular, high-order Taylor expansions of the solution (greater than two) will be considered in the framework of the Sensitivity Equation Method [61] (SEM) for unsteady aerodynamic applications, to improve the accuracy of mean and variance estimations. A second targeted topic in this context is the study of the uncertainty related to turbulence closure parameters, in the sequel of [150]. We aim at exploring the capability of the SEM approach to detect a change of flow topology, in case of detached flows. Our ambition is to contribute to the emergence of a new generation of simulation tools, which will provide solution densities rather than values, to tackle real-life uncertain problems. This task will also include a reflection about numerical schemes used to solve PDE systems, in the perspective of constructing a unified numerical framework able to account for exact geometries (isogeometric methods), uncertainty propagation and sensitivity analysis w.r.t. control parameters.

3.1.2. Optimization and control algorithms for systems governed by PDEs

The non-classical models described above are developed in the perspective of design improvement for real-life applications. Therefore, control and optimization algorithms are also developed in conjunction with these models. The focus here is on the methodological development and analysis of optimization algorithms for PDE systems in general, keeping in mind the application domains in the way the problems are mathematically formulated.

3.1.2.1. Sensitivity VS adjoint equation

Adjoint methods (achieved at continuous or discrete level) are now commonly used in industry for steady PDE problems. Our recent developments [141] have shown that the (discrete) adjoint method can be efficiently applied to cost gradient computations for time-evolving traffic flow on networks, thanks to the special structure of the associated linear systems and the underlying one dimensionality of the problem. However, this strategy is questionable for more complex (e.g. 2D/3D) unsteady problems, because it requires sophisticated and time-consuming check-pointing and/or re-computing strategies [56], [108] for the backward time integration of the adjoint variables. The sensitivity equation method (SEM) offers a promising alternative [89], [118], if the number of design parameters is moderate. Moreover, this approach can be employed for other goals, like fast evaluation of neighboring solutions or uncertainty propagation [90].
Regarding this topic, we intend to apply the continuous sensitivity equation method to challenging problems. In particular, in aerodynamics, multi-scale turbulence models like Large-Eddy Simulation (LES) [143] , Detached-Eddy Simulation (DES) [147] or Organized-Eddy Simulation (OES) [62], are more and more employed to analyse the unsteady dynamics of the flows around bluff-bodies, because they have the ability to compute the interactions of vortices at different scales, contrary to classical Reynolds-Averaged Navier-Stokes models. However, their use in design optimization is tedious, due to the long time integration required. In collaboration with turbulence specialists (M. Braza, CNRS - IMFT), we aim at developing numerical methods for effective sensitivity analysis in this context, and apply them to realistic problems, like the optimization of active flow control devices. Note that the use of SEM allows computing cost functional gradients at any time, which permits to construct new gradient-based optimization strategies like instantaneous-feedback method [120] or multiobjective optimization algorithm (see section below).

3.1.2.2. Multi-objective descent algorithms for multi-disciplinary, multi-point, unsteady optimization or robust-design

n differentiable optimization, multi-disciplinary, multi-point, unsteady optimization or robust-design can all be formulated as multi-objective optimization problems. In this area, we have proposed the *Multiple-Gradient*

Descent Algorithm (MGDA) to handle all criteria concurrently [91] [92]. Originally, we have stated a principle according which, given a family of local gradients, a descent direction common to all considered objective-functions simultaneously is identified, assuming the Pareto-stationarity condition is not satisfied. When the family is linearly-independent, we dispose of a direct algorithm. Inversely, when the family is linearly-dependent, a quadratic-programming problem should be solved. Hence, the technical difficulty is mostly conditioned by the number m of objective functions relative to the search space dimension n. In this respect, the basic algorithm has recently been revised [93] to handle the case where $m > n$, and even $m \gg n$, and is currently being tested on a test-case of robust design subject to a periodic time-dependent Navier-Stokes flow.

The multi-point situation is very similar and, being of great importance for engineering applications, will be treated at large.

Moreover, we intend to develop and test a new methodology for robust design that will include uncertainty effects. More precisely, we propose to employ MGDA to achieve an effective improvement of all criteria simultaneously, which can be of statistical nature or discrete functional values evaluated in confidence intervals of parameters. Some recent results obtained at ONERA [136] by a stochastic variant of our methodology confirm the viability of the approach. A PhD thesis has also been launched at ONERA/DADS.

Lastly, we note that in situations where gradients are difficult to evaluate, the method can be assisted by a meta-model [156].

3.1.2.3. Bayesian Optimization algorithms for efficient computation of general equilibria

Bayesian Optimization -BO- relies on Gaussian processes, which are used as emulators (or surrogates) of the black-box model outputs based on a small set of model evaluations. Posterior distributions provided by the Gaussian process are used to design acquisition functions that guide sequential search strategies that balance between exploration and exploitation. Such approaches have been transposed to frameworks other than optimization, such as uncertainty quantification. Our aim is to investigate how the BO apparatus can be applied to the search of general game equilibria, and in particular the classical Nash equilibrium (NE). To this end, we propose two complementary acquisition functions, one based on a greedy search approach and one based on the Stepwise Uncertainty Reduction paradigm [100]. Our proposal is designed to tackle derivative-free, expensive models, hence requiring very few model evaluations to converge to the solution.

3.1.2.4. Decentralized strategies for inverse problems

Most if not all the mathematical formulations of inverse problems (a.k.a. reconstruction, identification, data recovery, non destructive engineering,...) are known to be ill posed in the Hadamard sense. Indeed, in general, inverse problems try to fulfill (minimize) two or more very antagonistic criteria. One classical example is the Tikhonov regularization, trying to find artificially smoothed solutions close to naturally non-smooth data.

We consider here the theoretical general framework of parameter identification coupled to (missing) data recovery. Our aim is to design, study and implement algorithms derived within a game theoretic framework, which are able to find, with computational efficiency, equilibria between the "identification related players" and the "data recovery players". These two parts are known to pose many challenges, from a theoretical point of view, like the identifiability issue, and from a numerical one, like convergence, stability and robustness problems. These questions are tricky [47] and still completely open for systems like e.g. coupled heat and thermoelastic joint data and material detection.

CAGIRE Project-Team

3. Research Program

3.1. The scientific context

3.1.1. Computational fluid mechanics: modeling or not before discretizing ?

A typical continuous solution of the Navier-Stokes equations at sufficiently large values of the Reynolds number is governed by a wide spectrum of temporal and spatial scales closely connected with the turbulent nature of the flow. The term deterministic chaos employed by Frisch in his enlightening book [49] is certainly conveying most adequately the difficulty in analyzing and simulating this kind of flows. The broadness of the turbulence spectrum is directly controlled by the Reynolds number defined as the ratio between the inertial forces and the viscous forces. This number is not only useful to determine the transition from a laminar to a turbulent flow regime, it also indicates the range of scales of fluctuations that are present in the flow under consideration. Typically, for the velocity field and far from solid walls, the ratio between the largest scale (the integral length scale) and the smallest one (Kolmogorov scale) is proportional to $Re_t^{3/4}$ per dimension, where $Re_t^{3/4}$ is the turbulent Reynolds number, based on the length and velocity scales of the largest turbulent eddies. In addition, for internal flows, viscous effects near the solid walls yield a scaling proportional to Re_τ per dimension, where Re_τ is the friction Reynolds number. The smallest scales play a crucial role in the dynamics of the largest ones, which implies that an accurate framework for the computation of turbulent flows must take into account all the scales, which can lead to unrealistic computational costs in real-world applications. Thus, the usual practice to deal with turbulent flows is to choose between an a priori modeling (in most situations) or not (low Re number and rather simple configurations) before proceeding to the discretization step, followed by the simulation itself. If a modeling phase is on the agenda, then one has to choose again among the above-mentioned variety of approaches. The different simulation options and their date of availability for high-Reynolds-number applications are illustrated in Fig. 1 : simulation of turbulent flows can be achieved either by directly solving the Navier-Stokes equations (DNS) or by first applying to the equations a statistical averaging (RANS), a spatial filtering (LES), or a combination of these two operators (hybrid RANS/LES). The new terms brought about by the operator have to be modeled. From a computational point of view, the RANS approach is the least demanding, which explains why historically it has been the workhorse in both the academic and the industrial sectors, and it remains the standard approach nowadays for industrial design, except for very specific applications. It has permitted quite a substantial progress in the understanding of various phenomena such as turbulent combustion or heat transfer. Its inherent inability to provide a time-dependent information has led to promote in the last decade the recourse to either LES or DNS to supplement if not replace RANS. By simulating the large scale structures while modeling the smallest ones, assumed more isotropic, LES proved to be quite a breakthrough to fully take advantage of the increasing power of computers to study complex flow configurations. At the same time, DNS was gradually applied to geometries of increasing complexity (channel flows with values of Re_τ multiplied by 45 during the last 30 years, jets, turbulent premixed flames, among many others), and proved to be a formidable tool to **(i)** improve our knowledge on turbulent flows and **(ii)** test (i.e., validate or invalidate) and improve the modeling hypotheses inherently associated to the RANS and LES approaches. From a numerical point of view, due to the steady nature of the RANS equations, numerical accuracy is generally not ensured via the use of high-order schemes, but rather on careful grid convergence studies. In contrast, the high computational cost of LES or DNS makes necessary the use of highly-accurate numerical schemes in order to optimize the use of computational resources.

To the noticeable exception of the hybrid RANS-LES modeling, which is not yet accepted as a reliable tool for industrial design, as mentioned in the preamble of the Go4hybrid European program [0], a turbulence model represents turbulent mechanisms in the same way in the whole flow. Thus, depending on its intrinsic strengths

[0] https://cordis.europa.eu/project/rcn/109107/factsheet/en

and weaknesses, accuracy will be a rather volatile quantity, strongly dependent on the flow configuration. For instance, RANS is perfectly suited to attached boundary layers, but exhibits severe limitations in massively-separated flow regions. Therefore, the turbulence modeling and industrial design communities waver between the desire to continue to rely on the RANS approach, which is unrivaled in terms of computational cost, but is still not able to accurately represent all the complex phenomena; and the temptation to switch to LES, which outperforms RANS in many situations, but is prohibitively expensive in high-Reynolds number wall-bounded flows. In order to account for the limitations of the two approaches and to combine them for significantly improving the overall performance of the models, the hybrid RANS-LES approach has emerged during the last two decades as a viable, intermediate way, and we are definitely inscribing our project in this innovative field of research, with an original approach though, based on temporal filtering (Hybrid temporal LES, HTLES) rather than spatial filtering, and a systematic and progressive validation process against experimental data produced by the team.

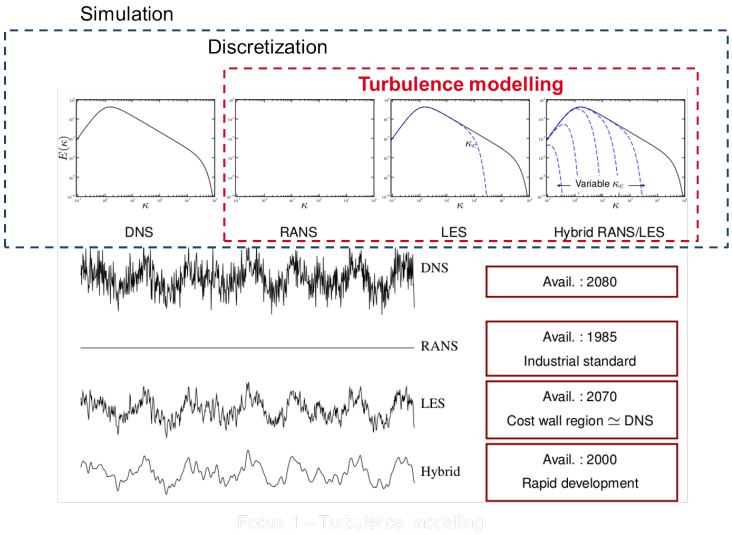

Figure 1. Schematic view of the different nested steps for turbulent flow simulation: from DNS to hybrid RANS-LES. The approximate dates at which the different approaches are or will be routinely used in the industry are indicated in the boxes on the right (extrapolations based on the present rate of increase in computer performances).

3.1.2. Computational fluid mechanics: high order discretization on unstructured meshes and efficient methods of solution

All the methods considered in the project are mesh-based methods: the computational domain is divided into cells, that have an elementary shape: triangles and quadrangles in two dimensions, and tetrahedra, hexahedra, pyramids, and prisms in three dimensions. If the cells are only regular hexahedra, the mesh is said to be structured. Otherwise, it is said to be unstructured. If the mesh is composed of more than one sort of elementary shape, the mesh is said to be hybrid. In the project, the numerical strategy is based on discontinuous Galerkin methods. These methods were introduced by Reed and Hill [60] and first studied by Lesaint and Raviart [56]. The extension to the Euler system with explicit time integration was mainly led by Shu, Cockburn and their collaborators. The steps of time integration and slope limiting were similar to high-order ENO schemes, whereas specific constraints given by the finite-element nature of the scheme were gradually solved for scalar conservation laws [44], [43], one dimensional systems [42], multidimensional scalar conservation laws [41], and multidimensional systems [45]. For the same system, we can also cite the work of [48], [53], which is

slightly different: the stabilization is made by adding a nonlinear term, and the time integration is implicit. In contrast to continuous Galerkin methods, the discretization of diffusive operators is not straightforward. This is due to the discontinuous approximation space, which does not fit well with the space function in which the diffusive system is well posed. A first stabilization was proposed by Arnold [34]. The first application of discontinuous Galerkin methods to Navier-Stokes equations was proposed in [39] by mean of a mixed formulation. Actually, this first attempt led to a non-compact computational stencil, and was later proved to be unstable. A compactness improvement was made in [40], which was later analyzed, and proved to be stable in a more unified framework [35]. The combination with the $k-\omega$ RANS model was made in [38]. As far as Navier-Stokes equations are concerned, we can also cite the work of [51], in which the stabilization is closer to the one of [35], the work of [57] on local time stepping, or the first use of discontinuous Galerkin methods for direct numerical simulation of a turbulent channel flow done in [46]. Discontinuous Galerkin methods became very popular because:

- They can be developed for any order of approximation.
- The computational stencil of one given cell is limited to the cells with which it has a common face. This stencil does not depend on the order of approximation. This is a pro, compared for example with high-order finite volumes, for which the number of neighbors required increases with the order of approximation.
- They can be developed for any kind of mesh, structured, unstructured, but also for aggregated grids [37]. This is a pro compared not only with finite-difference schemes, which can be developed only on structured meshes, but also compared with continuous finite-element methods, for which the definition of the approximation basis is not clear on aggregated elements.
- p-adaptivity is easier than with continuous finite elements, because neighboring elements having a different order are only weakly coupled.
- Upwinding is as natural as for finite volumes methods, which is a benefit for hyperbolic problems.
- As the formulation is weak, boundary conditions are naturally weakly formulated. This is a benefit compared with strong formulations, for example point centered formulation when a point is at the intersection of two kinds of boundary conditions.

For concluding this section, there already exists numerical schemes based on the discontinuous Galerkin method, which proved to be efficient for computing compressible viscous flows. Nevertheless, there remain many things to be improved, which include: efficient shock capturing methods for supersonic flows, high-order discretization of curved boundaries, low-Mach-number behavior of these schemes and combination with second-moment RANS closures. Another aspect that deserves attention is the computational cost of discontinuous Galerkin methods, due to the accurate representation of the solution, calling for a particular care of implementation for being efficient. We believe that this cost can be balanced by the strong memory locality of the method, which is an asset for porting on emerging many-core architectures.

3.1.3. Experimental fluid mechanics: a relevant tool for physical modeling and simulation development

With the considerable and constant development of computer performance, many people were thinking at the turn of the 21st century that in the short term, CFD would replace experiments, considered as too costly and not flexible enough. Simply flipping through scientific journals such as Journal of Fluid Mechanics, Combustion and Flame, Physics of Fluids or Journal of Computational Physics or through websites such that of Ercoftac [0] is sufficient to convince oneself that the recourse to experiments to provide either a quantitative description of complex phenomena or reference values for the assessment of the predictive capabilities of models and simulations is still necessary. The major change that can be noted though concerns the content of the interaction between experiments and CFD (understood in the broad sense). Indeed, LES or DNS assessment calls for the experimental determination of temporal and spatial turbulent scales, as well as time-resolved measurements and determination of single or multi-point statistical properties of the velocity field. Thus, the team methodology incorporates from the very beginning an experimental component that is operated in strong interaction with the modeling and simulation activities.

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

3.2. Research directions

3.2.1. Boundary conditions

3.2.1.1. Generating synthetic turbulence

A crucial point for any multi-scale simulation able to locally switch (in space or time) from a coarse to a fine level of description of turbulence, is the enrichment of the solution by fluctuations as physically meaningful as possible. Basically, this issue is an extension of the problem of the generation of realistic inlet boundary conditions in DNS or LES of subsonic turbulent flows. In that respect, the method of anisotropic linear forcing (ALF) we have developed in collaboration with EDF proved very encouraging, by its efficiency, its generality and simplicity of implementation. So, it seems natural, on the one hand, to extend this approach to the compressible framework and to implement it in AeroSol. On the other hand, we shall concentrate (in cooperation with EDF R&D in Chatou in the framework of a the CIFRE PhD of V. Duffal) on the theoretical link between the local variations of the scale of description of turbulence (e.g. a sudden variations in the size of the time filter) and the intensity of the ALF forcing, transiently applied to promote the development of missing fluctuating scales.

3.2.1.2. Stable and non reflecting boundary conditions

In aerodynamics, and especially for subsonic computations, handling inlet and outlet boundary conditions is a difficult issue. A significant amount of work has already been performed for second-order schemes for Navier-Stokes equations, see [59], [62] and the huge number of papers citing it. On the one hand, we believe that decisive improvements are necessary for higher-order schemes: indeed, the less dissipative the scheme is, the worse impact have the spurious reflections. For this purpose, we will first concentrate on the linearized Navier-Stokes system, and analyze the way to impose boundary conditions in a discontinuous Galerkin framework with a similar approach as in [50]. We will also try to extend the work of [63], which deals with Euler equations, to the Navier-Stokes equations.

3.2.2. Turbulence models and model agility

3.2.2.1. Extension of zero-Mach models to the compressible system

We shall develop in parallel our multi-scale turbulence modeling and the related adaptive numerical methods of AeroSol. Without prejudice to methods that will be on the podium in the future, a first step in this direction will be to extend to a compressible framework the continuous temporal hybrid RANS/LES method we have developed up to now in a Mach zero context.

3.2.2.2. Study of wall flows with and without mass or heat transfer at the wall: determination and validation of relevant criteria for hybrid turbulence models

In the targeted application domains, turbulence/wall interactions and heat transfer at the fluid-solid interface are physical phenomena whose numerical prediction is at the heart of the concerns of our industrial partners. For instance, for a jet engine manufacturer, being able to properly design the configuration of the cooling of the walls of its engine combustion chamber in the presence of thermoacoustic instabilities is based on the proper identification and a thorough understanding of the major mechanisms that drive the dynamics of the parietal transfer. Our objective is to take advantage of our analysis, experimental and computational tools to actively participate in the improvement of the collective knowledge of such kind of transfer. The flow configurations dealt with from the beginning of the project are those of subsonic, single-phase impinging jets or JICF (jets in crossflow) with the possible presence of an interacting acoustic wave. The issue of conjugate heat transfer at the wall will be also gradually investigated. The existing switchover criteria of the hybrid RANS/LES models will be tested on these flow configurations in order to determine their domain of validity. In parallel, the hydrodynamic instability modes of the JICF will be studied experimentally and theoretically (in cooperation with the SIAME laboratory) in order to determine the possibility to drive a change of instability regime (e.g., from absolute to convective) and thus to propose challenging flow conditions that would be relevant for the setting-up of an hybrid LES/DNS approach aimed at supplementing the hybrid RANS/LES approach.

3.2.2.3. Improvement of turbulence models

The production and subsequent use of DNS (AeroSol library) and experimental (MAVERIC bench) databases dedicated to the improvement of the physical models is a significant part of our activity. In that respect, our present capability of producing in-situ experimental data for simulation validation and flow analysis is clearly a strongly differentiating mark of our project. The analysis of the DNS and experimental data produced make the improvement of the hybrid RANS/LES approach possible. Our hybrid temporal LES (HTLES) method has a decisive advantage over all other hybrid RANS/LES approaches since it relies on a well-defined time-filtering formalism. This feature greatly facilitates the proper extraction from the databases of the various terms appearing in transport equations obtained at the different scales involved (e.g. from RANS to LES). But we would not be comprehensive in that matter if we were not questioning the relevance of any simulation-experiment comparisons. In other words, a central issue is the following question: are we comparing the same quantities between simulations and experiment? From an experimental point of view, the questions to be raised will be, among others, the possible difference in resolution between the experiment and the simulations, the similar location of the measurement points and simulation points, the acceptable level of random error associated to the necessary finite number of samples. In that respect, the recourse to uncertainty quantification techniques will be advantageously considered.

3.2.3. Development of an efficient implicit high-order compressible solver scalable on new architectures

As the flows simulated are very computationally demanding, we will maintain our efforts in the development of AeroSol in the following directions:

- Efficient implementation of the discontinuous Galerkin method.
- Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid.
- Porting on heterogeneous architectures.
- Implementation of models.

3.2.3.1. Efficient implementation of the discontinuous Galerkin method

In high-order discontinuous Galerkin methods, the unknown vector is composed of a concatenation of the unknowns in the cells of the mesh. An explicit residual computation is composed of three loops: an integration loop on the cells, for which computations in two different cells are independent, an integration loop on boundary faces, in which computations depend on data of one cell and on the boundary conditions, and an integration loop on the interior faces, in which computations depend on data of the two neighboring cells. Each of these loops is composed of three steps: the first step consists in interpolating data at the quadrature points; the second step in computing a nonlinear flux at the quadrature points (the physical flux for the cell loop, an upwind flux for interior faces or a flux adapted to the kind of boundary condition for boundary faces); and the third step in projecting the nonlinear flux on the degrees of freedom.

In this research direction, we propose to exploit the strong memory locality of the method (i.e., the fact that all the unknowns of a cell are stocked contiguously). This formulation can reduce the linear steps of the method (interpolation on the quadrature points and projection on the degrees of freedom) to simple matrix-matrix product which can be optimized. For the nonlinear steps, composed of the computation of the physical flux on the cells and of the numerical flux on the faces, we will try to exploit vectorization.

3.2.3.2. Implicit methods based on Jacobian-Free-Newton-Krylov methods and multigrid

For our computations of the IMPACT-AE project, we have used explicit time stepping. The time stepping is limited by the CFL condition, and in our flow, the time step is limited by the acoustic wave velocity. As the Mach number of the flow we simulated in IMPACT-AE was low, the acoustic time restriction is much lower than the turbulent time scale, which is driven by the velocity of the flow. We hope to have a better efficiency by using time implicit methods, for using a time step driven by the velocity of the flow.

Using implicit time stepping in compressible flows in particularly difficult, because the system is fully nonlinear, such that the nonlinear solving theoretically requires to build many times the Jacobian. Our experience in implicit methods is that the building of a Jacobian is very costly, especially in three dimensions and in a high-order framework, because the optimization of the memory usage is very difficult. That is why we propose to use a Jacobian-free implementation, based on [55]. This method consists in solving the linear steps of the Newton method by a Krylov method, which requires Jacobian-vector product. The smart idea of this method is to replace this product by an approximation based on a difference of residual, therefore avoiding any Jacobian computation. Nevertheless, Krylov methods are known to converge slowly, especially for the compressible system when the Mach number is low, because the system is ill-conditioned. In order to precondition, we propose to use an aggregation-based multigrid method, which consists in using the same numerical method on coarser meshes obtained by aggregation of the initial mesh. This choice is driven by the fact that multigrid methods are the only one to scale linearly [64], [65] with the number of unknowns in term of number of operations, and that this preconditioning does not require any Jacobian computation.

Beyond the technical aspects of the multigrid approach, which is challenging to implement, we are also interested in the design of an efficient aggregation. This often means to perform an aggregation based on criteria (anisotropy of the problem, for example) [58]. To this aim, we propose to extend the scalar analysis of [66] to a linearized version of the Euler and Navier-Stokes equations, and try to deduce an optimal strategy for anisotropic aggregation, based on the local characteristics of the flow. Note that discontinuous Galerkin methods are particularly well suited to h-p aggregation, as this kind of methods can be defined on any shape [37].

3.2.3.3. Porting on heterogeneous architectures

Until the beginning of the 2000s, the computing capacities have been improved by interconnecting an increasing number of more and more powerful computing nodes. The computing capacity of each node was increased by improving the clock speed, the number of cores per processor, the introduction of a separate and dedicated memory bus per processor, but also the instruction level parallelism, and the size of the memory cache. Even if the number of transistors kept on growing up, the clock speed improvement has flattened since the mid 2000s [61]. Already in 2003, [52] pointed out the difficulties for efficiently using the biggest clusters: "While these super-clusters have theoretical peak performance in the Teraflops range, sustained performance with real applications is far from the peak. Salinas, one of the 2002 Gordon Bell Awards was able to sustain 1.16 Tflops on ASCI White (less than 10% of peak)." From the current multi-core architectures, the trend is now to use many-core accelerators. The idea behind many-core is to use an accelerator composed of a lot of relatively slow and simplified cores for executing the most simple parts of the algorithm. The larger the part of the code executed on the accelerator, the faster the code may become. Therefore, it is necessary to work on the heterogeneous aspects of computations. These heterogeneities are intrinsic to our computations and have two sources. The first one is the use of hybrid meshes, which are necessary for using a locally-structured mesh in a boundary layer. As the different cell shapes (pyramids, hexahedra, prisms and tetrahedra) do not have the same number of degrees of freedom, nor the same number of quadrature points, the execution time on one face or one cell depends on its shape. The second source of heterogeneity are the boundary conditions. Depending on the kind of boundary conditions, user-defined boundary values might be needed, which induces a different computational cost. Heterogeneities are typically what may decrease efficiency in parallel if the workload is not well balanced between the cores. Note that heterogeneities were not dealt with in what we consider as one of the most advanced work on discontinuous Galerkin on GPU [54], as only straight simplicial cell shapes were addressed. For managing at best our heterogeneous computations on heterogeneous architectures, we propose to use the execution runtime StarPU [36]. For this, the discontinuous Galerkin algorithm will be reformulated in terms of a graph of tasks. The previous tasks on the memory management will be useful for that. The linear steps of the discontinuous Galerkin methods require also memory transfers, and one issue consists in determining the optimal task granularity for this step, i.e. the number of cells or face integrations to be sent in parallel on the accelerator. On top of that, the question of which device is the most appropriate to tackle such kind of tasks is to be discussed.

Last, we point out that the combination of shared-memory and distributed-memory parallel programming models is better suited than only the distributed-memory one for multigrid, because in a hybrid version, a wider part of the mesh shares the same memory, therefore making a coarser aggregation possible.

These aspects will benefit from a particularly stimulating environment in the Inria Bordeaux Sud Ouest center around high-performance computing, which is one of the strategic axes of the center.

3.2.3.4. Implementation of turbulence models in AeroSol and validation

We will gradually insert models developed in research direction 3.2.2.1 in the AeroSol library in which we develop methods for the DNS of compressible turbulent flows at low Mach number. Indeed, due to its formalism based on temporal filtering, the HTLES approach offers a consistent theoretical framework characterized by a continuous transition from RANS to DNS, even for complex flow configurations (e.g. without directions of spatial homogeneity). As for the discontinuous Galerkin method available presently in AeroSol, it is the best suited and versatile method able to meet the requirements of accuracy, stability and cost related to the local (varying) level of resolution of the turbulent flow at hand, regardless of its complexity. The first step in this direction was taken in 2017 during the internship of Axelle Perraud, who has implemented a turbulence model (k-ω-SST) in the Aerosol library.

3.2.4. Validation of the simulations: test flow configurations

To supplement whenever necessary the test flow configuration of MAVERIC and apart from configurations that could emerge in the course of the project, the following configurations for which either experimental data, simulation data or both have been published will be used whenever relevant for benchmarking the quality of our agile computations:

- The impinging turbulent jet (simulations).
- The ORACLES two-channel dump combustor developed in the European projects LES4LPP and MOLECULES.
- The non reactive single-phase PRECCINSTA burner (monophasic swirler), a configuration that has been extensively calculated in particular with the AVBP and Yales2 codes.
- The LEMCOTEC configuration (monophasic swirler + effusion cooling).
- The ONERA MERCATO two-phase injector configuration provided the question of confidentiality of the data is not an obstacle.
- Rotating turbulent flows with wall interaction and heat transfer.
- Turbulent flows with buoyancy.

CARDAMOM Project-Team

3. Research Program

3.1. Variational discrete asymptotic modelling

In many of the applications we consider, intermediate fidelity models are or can be derived using an asymptotic expansion for the relevant scale resolving PDEs, and eventually considering some averaged for of the resulting continuous equations. The resulting systems of PDEs are often very complex and their characterization, e.g. in terms of stability, unclear, or poor, or too complex to allow to obtain discrete analogy of the continuous properties. This makes the numerical approximation of these PDE systems a real challenge. Moreover, most of these models are often based on asymptotic expansions involving small geometrical scales. This is true for many applications considered here involving flows in/of thin layers (free surface waves, liquid films on wings generating ice layers, oxide flows in material cracks, etc). This asymptotic expansion is nothing else than a discretization (some sort of Taylor expansion) in terms of the small parameter. The actual discretization of the PDE system is another expansion in space involving as a small parameter the mesh size. What is the interaction between these two expansions ? Could we use the spatial discretization (truncation error) as means of filtering undesired small scales instead of having to explicitly derive PDEs for the large scales ? We will investigate in depth the relations between asymptotics and discretization by :

- comparing the asymptotic limits of discretized forms of the relevant scale resolving equations with the discretization of the analogous continuous asymptotic PDEs. Can we discretize a well understood system of PDEs instead of a less understood and more complex one ? ;
- study the asymptotic behaviour of error terms generated by coarse one-dimensional discretization in the direction of the “small scale”. What is the influence of the number of cells along the vertical direction, and of their clustering ? ;
- derive equivalent continuous equations (modified equations) for anisotropic discretizations in which the direction is direction of the “small scale” is approximated with a small number of cells. What is the relation with known asymptotic PDE systems ?

Our objective is to gain sufficient control of the interaction between discretization and asymptotics to be able to replace the coupling of several complex PDE systems by adaptive strongly anisotrotropic finite element approximations of relevant and well understood PDEs. Here the anisotropy is intended in the sense of having a specific direction in which a much poorer (and possibly variable with the flow conditions) polynomial approximation (expansion) is used. The final goal is, profiting from the availability of faster and cheaper computational platforms, to be able to automatically control numerical *and* physical accuracy of the model with the same techniques. This activity will be used to improve our modelling in coastal engineering as well as for de-anti icing systems, wave energy converters, composite materials (cf. next sections).

In parallel to these developments, we will make an effort in to gain a better understanding of continuous asymptotic PDE models. We will in particular work on improving, and possibly, simplifying their numerical approximation. An effort will be done in trying to embed in these more complex nonlinear PDE models discrete analogs of operator identities necessary for stability (see e.g. the recent work of [91], [96] and references therein).

3.2. High order discretizations on moving adaptive meshes

We will work on both the improvement of high order mesh generation and adaptation techniques, and the construction of more efficient, adaptive high order discretisation methods.

Concerning curved mesh generation, we will focus on two points. First propose a robust and automatic method to generate curved simplicial meshes for realistic geometries. The untangling algorithm we plan to develop is a hybrid technique that gathers a local mesh optimization applied on the surface of the domain and a linear elasticity analogy applied in its volume. Second we plan to extend the method proposed in [47] to hybrid meshes (prism/tetra).

For time dependent adaptation we will try to exploit as much as possible the use of $r-$adaptation techniques based on the solution of some PDE system for the mesh. We will work on enhancing the results of [3] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [106], [112], [61]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [47], and with improved algorithms to discretize accurately and fast the elliptic equations involved. For this we will explore different type of relaxation methods, including those proposed in [94], [99], [98] allowing to re-use high order discretizations techniques already used for the flow variables. All these modelling approaches for the mesh movement are based on some minimization argument, and do not allow easily to take into account explicitly properties such as e.g. the positivity of nodal volumes. An effort will be made to try to embed these properties, as well as to improve the control on the local mesh sizes obtained. Developments made in numerical methods for Lagrangian hydrodynamics and compressible materials may be a possible path for these objectives (see e.g. [72], [118], [117] and references therein). We will stretch the use of these techniques as much as we can, and couple them with remeshing algorithms based on local modifications plus conservative, high order, and monotone ALE (or other) remaps (cf. [48], [81], [119], [70] and references therein).
The development of high order schemes for the discretization of the PDE will be a major part of our activity. We will work from the start in an Arbitrary Lagrangian Eulerian setting, so that mesh movement will be easily accommodated, and investigate the following main points:

- the ALE formulation is well adapted both to handle moving meshes, and to provide conservative, high order, and monotone remaps between different meshes. We want to address the issue of cost-accuracy of adaptive mesh computations by exploring different degrees of coupling between the flow and the mesh PDEs. Initial experience has indicated that a clever coupling may lead to a considerable CPU time reduction for a given resolution [3]. This balance is certainly dependent on the nature of the PDEs, on the accuracy level sought, on the cost of the scheme, and on the time stepping technique. All these elements will be taken into account to try to provide the most efficient formulation ;
- the conservation of volume, and the subsequent preservation of constant mass-momentum-energy states on deforming domains is one of the most primordial elements of Arbitrary Lagrangian-Eulerian formulations. For complex PDEs as the ones considered here, of especially for some applications, there may be a competition between the conservation of e.g. mass, an the conservation of other constant states, as important as mass. This is typically the case for free surface flows, in which mass preservation is in competitions with the preservation of constant free surface levels [3]. Similar problems may arise in other applications. Possible solutions to this competition may come from super-approximation (use of higher order polynomials) of some of the data allowing to reduce (e.g. bathymetry) the error in the preservation of one of the competing quantities. This is similar to what is done in super-parametric approximations of the boundaries of an object immersed in the flow, except that in our case the data may enter the PDE explicitly and not only through the boundary conditions. Several efficient solutions for this issue will be investigated to obtain fully conservative moving mesh approaches:
- an issue related to the previous one is the accurate treatment of wall boundaries. It is known that even for standard lower order (second) methods, a higher order, curved, approximation of the boundaries may be beneficial. This, however, may become difficult when considering moving objects, as in the case e.g. of the study of the impact of ice debris in the flow. To alleviate this issue, we plan to follow on with our initial work on the combined use of immersed boundaries techniques with high order, anisotropic (curved) mesh adaptation. In particular, we will develop combined approaches involving high order hybrid meshes on fixed boundaries with the use of penalization techniques and immersed boundaries for moving objects. We plan to study the accuracy obtainable across discontinuous

functions with $r-$adaptive techniques, and otherwise use whenever necessary anisotropic meshes to be able to provide a simplified high order description of the wall boundary (cf. [90]). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body [97], [100]. An effort will be also made on improving the accuracy of these techniques using e.g. higher order approaches, either based on generalizations of classical splitting methods [82], or on some iterative Defect Correction method (see e.g. [63]) ;

- the proper treatment of different physics may be addressed by using mixed/hybrid schemes in which different variables/equations are approximated using a different polynomial expansion. A typical example is our work on the discretization of highly non-linear wave models [77] in which we have shown how to use a standard continuous Galerkin method for the elliptic equation/variable representative of the dispersive effects, while the underlying hyperbolic system is evolved using a (discontinuous) third order finite volume method. This technique will be generalized to other classes of discontinuous methods, and similar ideas will be used in other context to provide a flexible approximation. Such mathods have clear advantages in multiphase flows but not only. A typical example where such mixed methods are beneficial are flows involving different species and tracer equations, which are typically better treated with a discontinuous approximation. Another example is the use of this mixed approximation to describe the topography with a high order continuous polynomial even in discontinuous method. This allows to greatly simplify the numerical treatment of the bathymetric source terms ;
- the enhancement of stabilized methods based on some continuous finite element approximation will remain a main topic. We will further pursue the study on the construction of simplified stabilization operators which do not involve any contributions to the mass matrix. We will in particular generalize our initial results to higher order spatial approximations using cubature points, or Bezier polynomials, or also hierarchical approximations. This will also be combined with time dependent variants of the reconstruction techniques initially proposed by D. Caraeni [62], allowing to have a more flexible approach similar to the so-called P^nP^m method [75], [111]. How to localize these enhancements, and to efficiently perform local reconstructions/enrichment, as well as $p-$adaptation, and handling hanging nodes will also be a main line of work. A clever combination of hierarchical enrichment of the polynomials, with a constrained approximation will be investigated. All these developments will be combined with the shock capturing/positivity preserving construction we developed in the past. Other discontinuity resolving techniques will be investigated as well, such as face limiting techniques as those partially studied in [79] ;
- time stepping is an important issue, especially in presence of local mesh adaptation. The techniques we use will force us to investigate local and multilevel techniques. We will study the possibility constructing semi-implicit methods combining extrapolation techniques with space-time variational approaches. Other techniques will be considered, as multi-stage type methods obtained using Defect-Correction, Multi-step Runge-Kutta methods [59], as well as spatial partitioning techniques [87]. A major challenge will be to be able to guarantee sufficient locality to the time integration method to allow to efficiently treat highly refined meshes, especially for viscous reactive flows. Another challenge will be to embed these methods in the stabilized methods we will develop.

3.3. Coupled approximation/adaptation in parameter and physical space

As already remarked, classical methods for uncertainty quantification are affected by the so-called Curse-of-Dimensionality. Adaptive approaches proposed so far, are limited in terms of efficiency, or of accuracy. Our aim here is to develop methods and algorithms permitting a very high-fidelity simulation in the physical and in the stochastic space at the same time. We will focus on both non-intrusive and intrusive approaches.

Simple non-intrusive techniques to reduce the overall cost of simulations under uncertainty will be based on adaptive quadrature in stochastic space with mesh adaptation in physical space using error monitors related to the variance of to the sensitivities obtained e.g. by an ANOVA decomposition. For steady state problems,

remeshing using metric techniques is enough. For time dependent problems both mesh deformation and remeshing techniques will be used. This approach may be easily used in multiple space dimensions to minimize the overall cost of model evaluations by using high order moments of the properly chosen output functional for the adaptation (as in optimization). Also, for high order curved meshes, the use of high order moments and sensitivities issued from the UQ method or optimization provides a viable solution to the lack of error estimators for high order schemes.

Despite the coupling between stochastic and physical space, this approach can be made massively parallel by means of extrapolation/interpolation techniques for the high order moments, in time and on a reference mesh, guaranteeing the complete independence of deterministic simulations. This approach has the additional advantage of being feasible for several different application codes due to its non-intrusive character.
To improve on the accuracy of the above methods, intrusive approaches will also be studied. To propagate uncertainties in stochastic differential equations, we will use Harten's multiresolution framework, following [46]. This framework allows a reduction of the dimensionality of the discrete space of function representation, defined in a proper stochastic space. This reduction allows a reduction of the number of explicit evaluations required to represent the function, and thus a gain in efficiency. Moreover, multiresolution analysis offers a natural tool to investigate the local regularity of a function and can be employed to build an efficient refinement strategy, and also provides a procedure to refine/coarsen the stochastic space for unsteady problems. This strategy should allow to capture and follow all types of flow structures, and, as proposed in [46], allows to formulate a non-linear scheme in terms of compression capabilities, which should allow to handle non-smooth problems. The potential of the method also relies on its moderate intrusive behaviour, compared to e.g. spectral Galerkin projection, where a theoretical manipulation of the original system is needed.
Several activities are planned to generalize our initial work, and to apply it to complex flows in multiple (space) dimensions and with many uncertain parameters.

The first is the improvement of the efficiency. This may be achieved by means of anisotropic mesh refinement, and by experimenting with a strong parallelization of the method. Concerning the first point, we will investigate several anisotropic refinement criteria existing in literature (also in the UQ framework), starting with those already used in the team to adapt the physical grid. Concerning the implementation, the scheme formulated in [46] is conceived to be highly parallel due to the external cycle on the number of dimensions in the space of uncertain parameters. In principle, a number of parallel threads equal to the number of spatial cells could be employed. The scheme should be developed and tested for treating unsteady and discontinuous probability density function, and correlated random variables. Both the compression capabilities and the accuracy of the scheme (in the stochastic space) should be enhanced with a high-order multidimensional conservative and non-oscillatory polynomial reconstruction (ENO/WENO).

Another main objective is related to the use of multiresolution in both physical and stochastic space. This requires a careful handling of data and an updated definition of the wavelet. Until now, only a weak coupling has been performed, since the number of points in the stochastic space varies according to the physical space, but the number of points in the physical space remains unchanged. Several works exist on the multiresolution approach for image compression, but this could be the first time i in which this kind of approach would be applied at the same time in the two spaces with an unsteady procedure for refinement (and coarsening). The experimental code developed using these technologies will have to fully exploit the processing capabilities of modern massively parallel architectures, since there is a unique mesh to handle in the coupled physical/stochastic space.

3.4. Robust multi-fidelity modelling for optimization and certification

Due to the computational cost, it is of prominent importance to consider multi-fidelity approaches gathering high-fidelity and low-fidelity computations. Note that low-fidelity solutions can be given by both the use of surrogate models in the stochastic space, and/or eventually some simplified choices of physical models of some element of the system. Procedures which deal with optimization considering uncertainties for complex problems may require the evaluation of costly objective and constraint functions hundreds or even thousands of times. The associated costs are usually prohibitive. For these reason, the robustness of the optimal

solution should be assessed, thus requiring the formulation of efficient methods for coupling optimization and stochastic spaces. Different approaches will be explored. Work will be developed along three axes:

1. a robust strategy using the statistics evaluation will be applied separately, *i.e.* using only low or high-fidelity evaluations. Some classical optimization algorithms will be used in this case. Influence of high-order statistics and model reduction in the robust design optimization will be explored, also by further developing some low-cost methods for robust design optimization working on the so-called Simplex^2 method [68] ;
2. a multi-fidelity strategy by using in an efficient way low fidelity and high-fidelity estimators both in physical and stochastic space will be conceived, by using a Bayesian framework for taking into account model discrepancy and a PC expansion model for building a surrogate model ;
3. develop advanced methods for robust optimization. In particular, the Simplex^2 method will be modified for introducing a hierarchical refinement with the aim to reduce the number of stochastic samples according to a given design in an adaptive way.

This work is related to the activities foreseen in the EU contract MIDWEST, in the ANR LabCom project VIPER (currently under evaluation), in a joint project with DGA and VKI, in two projects under way with AIRBUS and SAFRAN-HERAKLES.

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, eventually including system uncertainties, 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. A part of the research activity is also devoted to take into account system uncertainties in the solving of inverse/optimization problems. At the interface of physics, mathematics, and computer science, Uncertainty Quantification (UQ) focuses on the development of frameworks and methods to characterize uncertainties in predictive computations. Uncertainties and errors arise at different stages of the numerical simulation. First, errors are introduced due to the physical simplifications in the mathematical modeling of the system investigated; other errors come from the numerical resolution of the mathematical model, due in particular to finite discretization and computations with finite accuracy and tolerance; finally, errors are due a limited knowledge of input quantities (parameters) appearing in the definition of the numerical model being solved.

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 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 universally satisfying solution (respecting 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.

In most cases, the used simplification result in a linearization of the inverse problem and therefore is usually valid only if the latter is weakly non-linear. The development of 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 is mainly motivated and inspired by recent advances in shape and topological optimization methods and in so-called sampling methods.

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.

The Team devotes a large effort focused on the formulation, implementation and validation of numerical methods for using scientific computing to drive experiments and available data (coming from models, simulation and experiments) by taking into account the system uncertainty. The team is also invested in exploiting the intimate relationship between optimisation and UQ to make Optimisation Under Uncertainty (OUU) tractable. A part of these activities is declined to the simulation of high-fidelity models for fluids, in three main fields, aerospace, energy and environment.

The Team is working on developing original UQ representations and algorithms to deal with complex and large scale models, having high dimensional input parameters with complexes influences. We are organizing our core research activities along different methodological UQ developments related to the challenges discussed above. Obviously, some efforts are shared by different initiatives or projects, and some of them include the continuous improvement of the non-intrusive methods constituting our software libraries. These actions are not detailed in the following, to focus the presentation on more innovative aspects, but we mentioned nonetheless the continuous developments and incorporation in our libraries of advanced sparse grid methods, sparsity promoting strategies and low rank methods.

An effort is dedicated to the efficient construction of surrogate models that are central in both forward and backward UQ problems, aiming at large-scale simulations relevant to engineering applications, with high dimensional input parameters.

Sensitivity analyses and other forward UQ problems (e.g., estimation of failure probabilities, rare events,. . .) depends on the input uncertainty model. Most often, for convenience or because of the lack of data, the independence of the uncertain inputs is assumed. In the Team, we are investigating approaches dedicated to a) the construction of uncertainty models that integrate the available information and expert knowledge(s) in a consistent and objective fashion. To this end, several mathematical frameworks are already available, e.g the maximum entropy principle, likelihood maximization and moment matching methods, but their application to real engineering problems remains scarce and their systematic use raises multiple challenges, both to construct the uncertainty model and to solve the related UQ problems (forward and backward). Because of the importance of the available data and expertise to build the model, the contributions of the Team in these areas depend on the needs and demands of end-users and industrial partners.

To mitigate computational complexity, the Team is exploring multi-fidelity approaches in the context of expensive simulations. We combine predictions of models with different levels of discretizations and physical simplifications to construct, at a controlled cost, reliable surrogate models of simulation outputs or directly objective functions and possibly constraints, to enable the resolution of robust optimization and stochastic inverse problems. Again, one difficulty to be addressed by the Team is the design of the computer experiments to obtain the best multi-fidelity model at the lowest cost (of for a prescribed computational budgets), with respect to the end use of the model. The last point is particularly challenging as it calls for accuracy for output values that are usually unknown a priori but must be estimated as the model construction proceeds.

ECUADOR Project-Team

3. Research Program

3.1. Algorithmic Differentiation

Participants: Laurent Hascoët, Valérie Pascual.

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

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

checkpointing General trade-off technique, used in adjoint AD, that trades duplicate execution of a part of the program to save some memory space that was used to save intermediate results.

Algorithmic Differentiation (AD) differentiates *programs*. The input of AD is a source program P that, given some $X \in \mathbb{R}^n$, returns some $Y = F(X) \in \mathbb{R}^m$, for a differentiable F. AD generates a new source program P' that, given X, computes some derivatives of F [2].

Any execution of P amounts to a sequence of instructions, which is identified with a composition of vector functions. Thus, if

$$\begin{array}{lll} P & \text{runs} & \{I_1; I_2; \cdots I_p;\}, \\ F & \text{then is} & f_p \circ f_{p-1} \circ \cdots \circ f_1, \end{array} \tag{2}$$

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

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

which can be mechanically written as a sequence of instructions I'_k. This can be generalized to higher level derivatives, Taylor series, etc. Combining the I'_k with the control of P yields P', and therefore this differentiation is piecewise.

The above computation of $F'(X)$, albeit simple and mechanical, can be prohibitively expensive on large codes. 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:

$$F'(X).\dot{X} = f'_p(X_{p-1}) \,.\, f'_{p-1}(X_{p-2}) \,.\, \cdots \,.\, f'_1(X_0) \,.\, \dot{X} \quad . \tag{4}$$

  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:

$$F'^*(X).\overline{Y} = f'^*_1(X_0).f'^*_2(X_1). \cdots .f'^*_{p-1}(X_{p-2}).f'^*_p(X_{p-1}).\overline{Y} \quad . \tag{5}$$

This expression is most efficiently computed from right to left, because matrix×vector products are cheaper than matrix×matrix products. This is the *adjoint mode* of AD, most effective for optimization, data assimilation [28], adjoint problems [21], or inverse problems.

Adjoint AD builds a very efficient program [24], which computes the gradient in a time independent from the number of parameters n. In contrast, computing the same gradient with the *tangent mode* would require running the tangent differentiated program n times.

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

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

3.2. Static Analysis and Transformation of programs

Participants: Laurent Hascoët, Valérie Pascual.

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

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

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

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

The most obvious example of a program transformation tool is certainly a compiler. Other examples are program translators, that go from one language or formalism to another, or optimizers, that transform a program to make it run better. AD is just one such transformation. These tools share the technological basis that lets them implement the sophisticated analyses [14] required. In particular there are common mathematical models to specify these analyses and analyze their properties.

An important principle is *abstraction*: the core of a compiler should not bother about syntactic details of the compiled program. The optimization and code generation phases must be independent from the particular input programming language. This is generally achieved using language-specific *front-ends*, language-independent *middle-ends*, and target-specific *back-ends*. In the middle-end, analysis can concentrate on the semantics of a reduced set of constructs. This analysis operates on an abstract representation of programs made of one *call graph*, whose nodes are themselves *flow graphs* whose nodes (*basic blocks*) contain abstract *syntax trees* for the individual atomic instructions. To each level are attached symbol tables, nested to capture scoping.

Static program analysis can be defined on this internal representation, which is largely language independent. The simplest analyses on trees can be specified with inference rules [17], [25], [15]. But many *data-flow analyses* are more complex, and better defined on graphs than on trees. Since both call graphs and flow graphs may be cyclic, these global analyses will be solved iteratively. *Abstract Interpretation* [18] 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 [31], [19] or pointers. Therefore, conservative *over-approximations* must be made, leading to derivative code less efficient than ideal.

3.3. Algorithmic Differentiation and Scientific Computing

Participants: Alain Dervieux, Laurent Hascoët, Bruno Koobus, Eléonore Gauci, Emmanuelle Itam, Olivier Allain, Stephen Wornom.

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

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

Scientific Computing provides reliable simulations of complex systems. For example it is possible to *simulate* the steady or unsteady 3D air flow around a plane that captures the physical phenomena of shocks and turbulence. Next comes *optimization*, one degree higher in complexity because it repeatedly simulates and applies gradient-based optimization steps until an optimum is reached. The next sophistication is *robustness*, that detects undesirable solutions which, although maybe optimal, are very sensitive to uncertainty on design parameters or on manufacturing tolerances. This makes second derivative come into play. Similarly *Uncertainty Quantification* can use second derivatives to evaluate how uncertainty on the simulation inputs imply uncertainty on its outputs.

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

- One can write an *adjoint system* of mathematical equations, then discretize it and program it by hand. This is time consuming. Although this looks mathematically sound [21], this does not provide the gradient of the discretized function itself, thus degrading the final convergence of gradient-descent optimization.
- One can apply adjoint AD (*cf*3.1) on the program that discretizes and solves the direct system. This gives exactly the adjoint of the discrete function computed by the program. Theoretical results [20] 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 [26], [29] to reduce memory usage.

If for instance the model is steady, or when the computation uses a Fixed-Point iteration, tradeoffs exist between these two extremes [22], [16] that combine low storage consumption with possible automated adjoint generation. We advocate incorporating them into the AD model and into the AD tools.

ELAN Team

3. Research Program

3.1. Discrete modeling of slender elastic structures

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

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

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

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

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

3.2. Discrete modeling of frictional contact

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

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

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

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

3.2.1. Optimized algorithms for large nodal systems in frictional contact

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

3.2.2. Continuum modeling of large fiber assemblies

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

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

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

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

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

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

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

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

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

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

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

3.3.2. Static inversion of physical objects from geometrical poses

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

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

3.3.3. Dynamic inversion of physical objects from geometrical poses

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

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

3.3.4. Experimental validation with respect to real data

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

GAMMA3 Project-Team (section vide)

MATHERIALS Project-Team

3. Research Program

3.1. Research Program

Our group, originally only involved in electronic structure computations, continues to focus on many numerical issues in quantum chemistry, but now expands its expertise to cover several related problems at larger scales, such as molecular dynamics problems and multiscale problems. The mathematical derivation of continuum energies from quantum chemistry models is one instance of a long-term theoretical endeavour.

3.1.1. Electronic structure of large systems

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

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

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

As the size of the systems one wants to study increases, more efficient numerical techniques need to be resorted to. In computational chemistry, the typical scaling law for the complexity of computations with respect to the size of the system under study is N^3, N being for instance the number of electrons. The Holy Grail in this respect is to reach a linear scaling, so as to make possible simulations of systems of practical interest in biology or material science. Efforts in this direction must address a large variety of questions such as

- how can one improve the nonlinear iterations that are the basis of any *ab initio* models for computational chemistry?
- how can one more efficiently solve the inner loop which most often consists in the solution procedure for the linear problem (with frozen nonlinearity)?
- how can one design a sufficiently small variational space, whose dimension is kept limited while the size of the system increases?

An alternative strategy to reduce the complexity of *ab initio* computations is to try to couple different models at different scales. Such a mixed strategy can be either a sequential one or a parallel one, in the sense that

- in the former, the results of the model at the lower scale are simply used to evaluate some parameters that are inserted in the model for the larger scale: one example is the parameterized classical molecular dynamics, which makes use of force fields that are fitted to calculations at the quantum level;
- while in the latter, the model at the lower scale is concurrently coupled to the model at the larger scale: an instance of such a strategy is the so called QM/MM coupling (standing for Quantum Mechanics/Molecular Mechanics coupling) where some part of the system (typically the reactive site of a protein) is modeled with quantum models, that therefore accounts for the change in the electronic structure and for the modification of chemical bonds, while the rest of the system (typically the inert part of a protein) is coarse grained and more crudely modeled by classical mechanics.

The coupling of different scales can even go up to the macroscopic scale, with methods that couple a microscopic representation of matter, or at least a mesoscopic one, with the equations of continuum mechanics at the macroscopic level.

3.1.2. Computational Statistical Mechanics

The orders of magnitude used in the microscopic representation of matter are far from the orders of magnitude of the macroscopic quantities we are used to: The number of particles under consideration in a macroscopic sample of material is of the order of the Avogadro number $\mathcal{N}_A \sim 6 \times 10^{23}$, the typical distances are expressed in Å (10^{-10} m), the energies are of the order of $k_{\mathrm{B}}T \simeq 4 \times 10^{-21}$ J at room temperature, and the typical times are of the order of 10^{-15} s.

To give some insight into such a large number of particles contained in a macroscopic sample, it is helpful to compute the number of moles of water on earth. Recall that one mole of water corresponds to 18 mL, so that a standard glass of water contains roughly 10 moles, and a typical bathtub contains 10^5 mol. On the other hand, there are approximately 10^{18} m^3 of water in the oceans, *i.e.*7×10^{22} mol, a number comparable to the Avogadro number. This means that inferring the macroscopic behavior of physical systems described at the microscopic level by the dynamics of several millions of particles only is like inferring the ocean's dynamics from hydrodynamics in a bathtub...

For practical numerical computations of matter at the microscopic level, following the dynamics of every atom would require simulating $\mathcal{N}_A$ atoms and performing $\mathrm{O}(10^{15})$ time integration steps, which is of course impossible! These numbers should be compared with the current orders of magnitude of the problems that can be tackled with classical molecular simulation, where several millions of atoms only can be followed over time scales of the order of a few microseconds.

Describing the macroscopic behavior of matter knowing its microscopic description therefore seems out of reach. Statistical physics allows us to bridge the gap between microscopic and macroscopic descriptions of matter, at least on a conceptual level. The question is whether the estimated quantities for a system of N particles correctly approximate the macroscopic property, formally obtained in the thermodynamic limit $N \to +\infty$ (the density being kept fixed). In some cases, in particular for simple homogeneous systems, the macroscopic behavior is well approximated from small-scale simulations. However, the convergence of the estimated quantities as a function of the number of particles involved in the simulation should be checked in all cases.

Despite its intrinsic limitations on spatial and timescales, molecular simulation has been used and developed over the past 50 years, and its number of users keeps increasing. As we understand it, it has two major aims nowadays.

First, it can be used as a *numerical microscope*, which allows us to perform "computer" experiments. This was the initial motivation for simulations at the microscopic level: physical theories were tested on computers. This use of molecular simulation is particularly clear in its historic development, which was triggered and sustained by the physics of simple liquids. Indeed, there was no good analytical theory for these systems, and the observation of computer trajectories was very helpful to guide the physicists' intuition about what was happening in the system, for instance the mechanisms leading to molecular diffusion. In particular, the pioneering works on Monte-Carlo methods by Metropolis *et al.*, and the first molecular dynamics simulation of Alder and Wainwright were performed because of such motivations. Today, understanding the behavior of matter at the microscopic level can still be difficult from an experimental viewpoint (because of the high resolution required, both in time and in space), or because we simply do not know what to look for! Numerical simulations are then a valuable tool to test some ideas or obtain some data to process and analyze in order to help assessing experimental setups. This is particularly true for current nanoscale systems.

Another major aim of molecular simulation, maybe even more important than the previous one, is to compute macroscopic quantities or thermodynamic properties, typically through averages of some functionals of the system. In this case, molecular simulation is a way to obtain *quantitative* information on a system, instead of resorting to approximate theories, constructed for simplified models, and giving only qualitative answers. Sometimes, these properties are accessible through experiments, but in some cases only numerical

computations are possible since experiments may be unfeasible or too costly (for instance, when high pressure or large temperature regimes are considered, or when studying materials not yet synthesized). More generally, molecular simulation is a tool to explore the links between the microscopic and macroscopic properties of a material, allowing one to address modelling questions such as "Which microscopic ingredients are necessary (and which are not) to observe a given macroscopic behavior?"

3.1.3. Homogenization and related problems

Over the years, the project-team has developed an increasing expertise on how to couple models written at the atomistic scale with more macroscopic models, and, more generally, an expertise in multiscale modelling for materials science.

The following observation motivates the idea of coupling atomistic and continuum representation of materials. In many situations of interest (crack propagation, presence of defects in the atomistic lattice, ...), using a model based on continuum mechanics is difficult. Indeed, such a model is based on a macroscopic constitutive law, the derivation of which requires a deep qualitative and quantitative understanding of the physical and mechanical properties of the solid under consideration. For many solids, reaching such an understanding is a challenge, as loads they are subjected to become larger and more diverse, and as experimental observations helping designing such models are not always possible (think of materials used in the nuclear industry). Using an atomistic model in the whole domain is not possible either, due to its prohibitive computational cost. Recall indeed that a macroscopic sample of matter contains a number of atoms on the order of 10^{23}. However, it turns out that, in many situations of interest, the deformation that we are looking for is not smooth in *only a small part* of the solid. So, a natural idea is to try to take advantage of both models, the continuum mechanics one and the atomistic one, and to couple them, in a domain decomposition spirit. In most of the domain, the deformation is expected to be smooth, and reliable continuum mechanics models are then available. In the rest of the domain, the expected deformation is singular, so that one needs an atomistic model to describe it properly, the cost of which remains however limited as this region is small.

From a mathematical viewpoint, the question is to couple a discrete model with a model described by PDEs. This raises many questions, both from the theoretical and numerical viewpoints:

- first, one needs to derive, from an atomistic model, continuum mechanics models, under some regularity assumptions that encode the fact that the situation is smooth enough for such a macroscopic model to provide a good description of the materials;
- second, couple these two models, e.g. in a domain decomposition spirit, with the specificity that models in both domains are written in a different language, that there is no natural way to write boundary conditions coupling these two models, and that one would like the decomposition to be self-adaptive.

More generally, the presence of numerous length scales in material science problems represents a challenge for numerical simulation, especially when some *randomness* is assumed on the materials. It can take various forms, and includes defects in crystals, thermal fluctuations, and impurities or heterogeneities in continuous media. Standard methods available in the literature to handle such problems often lead to very costly computations. Our goal is to develop numerical methods that are more affordable. Because we cannot embrace all difficulties at once, we focus on a simple case, where the fine scale and the coarse-scale models can be written similarly, in the form of a simple elliptic partial differential equation in divergence form. The fine scale model includes heterogeneities at a small scale, a situation which is formalized by the fact that the coefficients in the fine scale model vary on a small length scale. After homogenization, this model yields an effective, macroscopic model, which includes no small scale. In many cases, a sound theoretical groundwork exists for such homogenization results. The difficulty stems from the fact that the models generally lead to prohibitively costly computations. For such a case, simple from the theoretical viewpoint, our aim is to focus on different practical computational approaches to speed-up the computations. One possibility, among others, is to look for specific random materials, relevant from the practical viewpoint, and for which a dedicated approach can be proposed, that is less expensive than the general approach.

MEMPHIS Project-Team

3. Research Program

3.1. Reduced-order models

Massive parallelization and rethinking of numerical schemes will allow the use of mathematical models for a broader class of physical problems. For industrial applications, there is an increasing need for rapid and reliable numerical simulators to tackle design and control tasks. To provide a concrete example, in the design process of an aircraft, the flight conditions and manoeuvres, which provide the largest aircraft loads, are not known *a priori*. Therefore, the aerodynamic and inertial forces are calculated for a large number of conditions to give an estimate of the maximum loads, and hence stresses, that the structure of the detailed aircraft design might experience in service. As a result, the number of simulations required for a realistic design problem could easily be in the order of tens of millions. Even with simplistic models of the aircraft behavior this is an unfeasible number of separate simulations. However, engineering experience is used to identify the most likely critical load conditions, meaning that approximately hundreds of thousands simulations are required for conventional aircraft configurations. Furthermore, these analyses have to be repeated every time that there is an update in the aircraft structure.

Compared to existing approaches for ROMs [32], our interest will be focused on two axes. On the one hand, we start from the consideration that small, highly nonlinear scales are typically concentrated in limited spatial regions of the full simulation domain. So for example, in the flow past a wing, the highly non-linear phenomena take place in the proximity of the walls at the scale of a millimeter, for computational domains that are of the order of hundreds of meters. Based on these considerations, we propose in [15] a multi-scale model where the large scales are described by far-field models based on ROMs and the small scales are simulated by high-fidelity models. The whole point for this approach is to optimally decouple the far field from the near field.

A second characterizing feature of our ROM approach is non-linear interpolation. We start from the consideration that dynamical models derived from the projection of the PDE model in the reduced space are neither stable to numerical integration nor robust to parameter variation when hard non-linear multi-scale phenomena are considered.

However, thanks to Proper Orthogonal Decomposition (POD) [38], [44], [28] we can accurately approximate large solution databases using a low-dimensional base. Recent techniques to investigate the temporal evolution of the POD modes (Koopman modes [39], [26], Dynamic Mode Decomposition [42]) and allow a dynamic discrimination of the role played by each of them. This in turn can be exploited to interpolate between modes in parameter space, thanks to ideas relying on optimal transportation [46], [29] that we have started developing in the FP7 project FFAST and H2020 AEROGUST.

3.2. Hierarchical Cartesian schemes

We intend to conceive schemes that will simplify the numerical approximation of problems involving complex unsteady objects together with multi-scale physical phenomena. Rather than using extremely optimized but non-scalable algorithms, we adopt robust alternatives that bypass the difficulties linked to grid generation. Even if the mesh problem can be tackled today thanks to powerful mesh generators, it still represents a severe difficulty, in particular when highly complex unsteady geometries need to be dealt with. Industrial experience and common practice shows that mesh generation accounts for about 20% of overall analysis time, whereas creation of a simulation-specific geometry requires about 60%, and only 20% of overall time is actually devoted to analysis. The methods that we develop bypass the generation of tedious geometrical models by automatic implicit geometry representation and hierarchical Cartesian schemes.

The approach that we plan to develop combines accurate enforcement of unfitted boundary conditions with adaptive octree and overset grids. The core idea is to use an octree/overset mesh for the approximation of the solution fields, while the geometry is captured by level set functions [43], [37] and boundary conditions are imposed using appropriate interpolation methods [25], [45], [41]. This eliminates the need for boundary-conforming meshes that require time-consuming and error-prone mesh generation procedures, and opens the door for simulation of very complex geometries. In particular, it will be possible to easily import the industrial geometry and to build the associated level set function used for simulation.

Hierarchical octree grids offer several considerable advantages over classical adaptive mesh refinement for body-fitted meshes, in terms of data management, memory footprint and parallel HPC performance. Typically, when refining unstructured grids, like for example tetrahedral grids, it is necessary to store the whole data tree corresponding to successive subdivisions of the elements and eventually recompute the full connectivity graph. In the linear octree case that we develop, only the tree leaves are stored in a linear array, with a considerable memory advantage. The mapping between the tree leaves and the linear array as well as the connectivity graph is efficiently computed thanks to an appropriate space-filling curve. Concerning parallelization, linear octrees guarantee a natural load balancing thanks to the linear data structure, whereas classical unstructured meshes require sophisticated (and moreover time consuming) tools to achieve proper load distribution (SCOTCH, METIS etc.). Of course, using unfitted hierarchical meshes requires further development and analysis of methods to handle the refinement at level jumps in a consistent and conservative way, accuracy analysis for new finite-volume or finite-difference schemes, efficient reconstructions at the boundaries to recover appropriate accuracy and robustness. These subjects, that are currently virtually absent at Inria, are among the main scientific challenges of our team.

MEPHYSTO-POST Team

3. Research Program

3.1. Time asymptotics: Stationary states, solitons, and stability issues

The team investigates existence of solitons and their link with the global dynamical behavior for nonlocal problems such as that of the Gross–Pitaevskii (GP) equation which arises in models of dipolar gases. These models, in general, also introduce nonzero boundary conditions which constitute an additional theoretical and numerical challenge. Numerous results are proved for local problems, and numerical simulations allow to verify and illustrate them, as well as making a link with physics. However, most fundamental questions are still open at the moment for nonlocal problems.

The nonlinear Schrödinger (NLS) equation finds applications in numerous fields of physics. We concentrate, in a continued collaboration with our colleagues from the physics department (PhLAM) of the Université de Lille (UdL), in the framework of the Laboratoire d'Excellence CEMPI, on its applications in nonlinear optics and cold atom physics. Issues of orbital stability and modulational instability are central here.

Another typical example of problems that the team wishes to address concerns the LL equation, which describes the dynamics of the spin in ferromagnetic materials. This equation is a fundamental model in the magnetic recording industry [33] and solitons in magnetic media are of particular interest as a mechanism for data storage or information transfer [34]. It is a quasilinear PDE involving a function that takes values on the unit sphere $\mathbb{S}^2$ of $\mathbb{R}^3$. Using the stereographic projection, it can be seen as a quasilinear Schrödinger equation and the questions about the solitons, their dynamics and potential blow-up of solutions evoked above are also relevant in this context. This equation is less understood than the NLS equation: even the Cauchy theory is not completely done [28], [25]. In particular, the geometry of the target sphere imposes nonvanishing boundary conditions; even in dimension one, there are kink-type solitons having different limits at $\pm\infty$.

3.2. Derivation of macroscopic laws from microscopic dynamics

The team investigates, from a microscopic viewpoint, the dynamical mechanism at play in the phenomenon of relaxation towards thermal equilibrium for large systems of interacting particles. For instance, a first step consists in giving a rigorous proof of the fact that a particle repeatedly scattering of random obstacles through a Hamiltonian scattering process will eventually reach thermal equilibrium, thereby completing previous work in this direction by the team. As a second step, similar models as the ones considered classically will be defined and analysed in the quantum mechanical setting, and more particularly in the setting of quantum optics.

Another challenging problem is to understand the interaction of large systems with the boundaries, which is responsible for most energy exchanges (forcing and dissipation), even though it is concentrated in very thin layers. The presence of boundary conditions to evolution equations sometimes lacks understanding from a physical and mathematical point of view. In order to legitimate the choice done at the macroscopic level of the mathematical definition of the boundary conditions, we investigate systems of atoms (precisely chains of oscillators) with different local microscopic defects. We apply our recent techniques to understand how anomalous (in particular fractional) diffusive systems interact with the boundaries. For instance, the powerful tool given by Wigner functions that we already used has been successfully applied to the derivation of anomalous behaviors in open systems (for instance in [67]). The next step consists in developing an extension of that tool to deal with bounded systems provided with fixed boundaries. We also intend to derive anomalous diffusion by adding long range interactions to diffusive models. There are very few rigorous results in this direction. Finally, we aim at obtaining from a microscopic description the fractional porous medium equation (FPME), a nonlinear variation of the fractional diffusion equation, involving the fractional Laplacian instead of the usual one. Its rigorous study carries out many mathematical difficulties in treating at the same time the nonlinearity and fractional diffusion.

3.3. Numerical methods: analysis and simulations

The team addresses both questions of precision and numerical cost of the schemes for the numerical integration of nonlinear evolution PDEs, such as the NLS equation. In particular, we to develop, study and implement numerical schemes with high order that are more efficient. We also to contribute to the design and analysis of schemes with appropriate qualitative properties. These properties may as well be "asymptotic preserving" properties, energy-preserving properties, or convergence to an equilibrium properties. Other numerical goals of the team include the numerical simulation of standing waves of nonlinear nonlocal GP equations. We also keep on developing numerical methods to efficiently simulate and illustrate theoretical results on instability, in particular in the context of the modulational instability in optical fibers, where we study the influence of randomness in the physical parameters of the fibers.

MINGUS Project-Team

3. Research Program

3.1. Research Program

The MINGUS project is devoted to the mathematical and numerical analysis of models arising in plasma physics and nanotechnology. The main goal is to construct and analyze numerical methods for the approximation of PDEs containing multiscale phenomena. Specific multiscale numerical schemes will be proposed and analyzed in different regimes (namely highly-oscillatory and dissipative). The ultimate goal is to dissociate the physical parameters (generically denoted by ε) from the numerical parameters (generically denoted by h) with a uniform accuracy. Such a task requires mathematical prerequisite of the PDEs.

Then, for a given stiff (highly-oscillatory or dissipative) PDE, the methodology of the MINGUS team will be the following

- Mathematical study of the asymptotic behavior of multiscale models.
  This part involves averaging and asymptotic analysis theory to derive asymptotic models, but also long-time behavior of the considered models.
- Construction and analysis of multiscale numerical schemes.
  This part is the core of the project and will be deeply inspired for the mathematical prerequisite. In particular, our ultimate goal is the design of *Uniformly Accurate* (UA) schemes, whose accuracy is independent of ε.
- Validation on physically relevant problems.
  The last goal of the MINGUS project is to validate the new numerical methods, not only on toy problems, but also on realistic models arising in physics of plasmas and nanotechnologies. We will benefit from the Selalib software library which will help us to scale-up our new numerical methods to complex physics.

3.1.1. Dissipative problems

In the dissipative context, the asymptotic analysis is quite well understood in the deterministic case and multiscale numerical methods have been developed in the last decades. Indeed, the so-called Asymptotic-Preserving schemes has retained a lot of attention all over the world, in particular in the context of collisional kinetic equations. But, there is still a lot of work to do if one is interesting in the derivation high order asymptotic models, which enable to capture the original solution for all time. Moreover, this analysis is still misunderstood when more complex systems are considered, involving non homogeneous relaxation rates or stochastic terms for instance. Following the methodology we aim at using, we first address the mathematical analysis before deriving multiscale efficient numerical methods.

A simple model of dissipative systems is governed by the following differential equations

$$\left\{ \begin{array}{rcll} \dfrac{dx^\varepsilon(t)}{dt} & = & \mathcal{G}(x^\varepsilon(t), y^\varepsilon(t)), & x^\varepsilon(0) = x_0, \\ \dfrac{dy^\varepsilon(t)}{dt} & = & -\dfrac{y^\varepsilon(t)}{\varepsilon} + \mathcal{H}(x^\varepsilon(t), y^\varepsilon(t)), & y^\varepsilon(0) = y_0, \end{array} \right. \tag{6}$$

for given initial condition $(x_0, y_0) \in \mathbb{R}^2$ and given smooth functions $\mathcal{G}, \mathcal{H}$ which possibly involve stochastic terms.

3.1.1.1. Asymptotic analysis of dissipative PDEs (F. Castella, P. Chartier, A. Debussche, E. Faou, M. Lemou)

Derivation of asymptotic problems

Our main goal is to analyze the asymptotic behavior of dissipative systems of the form (3) when ε goes to zero. The *center manifold theorem* [35] is of great interest but is largely unsatisfactory from the following points of view

- a constructive approach of h and x_0^ε is clearly important to identify the high-order asymptotic models: this would require expansions of the solution by means of B-series or word-series [37] allowing the derivation of error estimates between the original solution and the asymptotic one.
- a better approximation of the transient phase is strongly required to capture the solution for small time: extending the tools developed in averaging theory, the main goal is to construct a suitable change of variable which enables to approximate the original solution for all time.

Obviously, even at the ODE level, a deep mathematical analysis has to be performed to understand the asymptotic behavior of the solution of (3). But, the same questions arise at the PDE level. Indeed, one certainly expects that dissipative terms occurring in collisional kinetic equations (2) may be treated theoretically along this perspective. The key new point indeed is to see the center manifold theorem as a change of variable in the space on unknowns, while the standard point of view leads to considering the center manifold as an asymptotic object.

Stochastic PDEs
We aim at analyzing the asymptotic behavior of stochastic collisional kinetic problems, that is equation of the type (2). The noise can describe creation or absorption (as in (2)), but it may also be a forcing term or a random magnetic field. In the parabolic scaling, one expect to obtain parabolic SPDEs at the limit. More precisely, we want to understand the fluid limits of kinetic equations in the presence of noise. The noise is smooth and non delta correlated. It contains also a small parameter and after rescaling converges formally to white noise. Thus, this adds another scale in the multiscale analysis. Following the pioneering work [38], some substantial progresses have been done in this topic.

More realistic problems may be addressed such as high field limit describing sprays, or even hydrodynamic limit. The full Boltzmann equation is a very long term project and we wish to address simpler problems such as convergences of BGK models to a stochastic Stokes equation.

The main difficulty is that when the noise acts as a forcing term, which is a physically relevant situation, the equilibria are affected by the noise and we face difficulties similar to that of high field limit problems. Also, a good theory of averaging lemma in the presence of noise is lacking. The methods we use are generalization of the perturbed test function method to the infinite dimensional setting. We work at the level of the generator of the infinite dimensional process and prove convergence in the sense of the martingale problems. A further step is to analyse the speed of convergence. This is a prerequisite if one wants to design efficient schemes. This requires more refined tools and a good understanding of the Kolmogorov equation.

3.1.1.2. Numerical schemes for dissipative problems (All members)

The design of numerical schemes able to reproduce the transition from the microscopic to macroscopic scales largely matured with the emergence of the Asymptotic Preserving schemes which have been developed initially for collisional kinetic equations (actually, for solving (2) when $\beta \to 0$). Several techniques have flourished in the last decades. As said before, AP schemes entail limitations which we aim at overcoming by deriving

- AP numerical schemes whose numerical cost diminishes as $\beta \to 0$,
- Uniformly accurate numerical schemes, whose accuracy is independent of β.

Time diminishing methods
The main goal consists in merging Monte-Carlo techniques [33] with AP methods for handling *automatically* multiscale phenomena. As a result, we expect that the cost of the so-obtained method decreases when the asymptotic regime is approached; indeed, in the collisional (i.e. dissipative) regime, the deviational part becomes negligible so that a very few number of particles will be generated to sample it. A work in this direction has been done by members of the team.

We propose to build up a method which permits to realize the transition from the microscopic to the macroscopic description without domain decomposition strategies which normally oblige to fix and tune an interface in the physical space and some threshold parameters. Since it will permit to go over domain decomposition and AP techniques, this approach is a very promising research direction in the numerical approximation of multiscale kinetic problems arising in physics and engineering.

Uniformly accurate methods
To overcome the accuracy reduction observed in AP schemes for intermediate regimes, we intend to construct and analyse multiscale numerical schemes for (3) whose error is uniform with respect to ε. The construction of such a scheme requires a deep mathematical analysis as described above. Ideally one would like to develop schemes that preserve the center manifold (without computing the latter!) as well as schemes that resolve numerically the stiffness induced by the fast convergence to equilibrium (the so-called transient phase). First, our goal is to extend the strategy inspired by the central manifold theorem in the ODE case to the PDE context, in particular for collisional kinetic equations (2) when $\beta \to 0$. The design of Uniformly Accurate numerical schemes in this context would require to generalize two-scale techniques introduced in the framework of highly-oscillatory problems [36].

Multiscale numerical methods for stochastic PDEs
AP schemes have been developed recently for kinetic equations with noise in the context of Uncertainty Quantification UQ [41]. These two aspects (multiscale and UQ) are two domains which usually come within the competency of separate communities. UQ has drawn a lot of attention recently to control the propagation of data pollution; undoubtedly UQ has a lot of applications and one of our goals will be to study how sources of uncertainty are amplified or not by the multiscale character of the model. We also wish to go much further and by developing AP schemes when the noise is also rescaled and the limit is a white noise driven SPDE, as described in section (3.1.1.1). For simple nonlinear problem, this should not present much difficulties but new ideas will definitely be necessary for more complicated problems when noise deeply changes the asymptotic equation.

3.1.2. Highly-oscillatory problems

As a generic model for highly-oscillatory systems, we will consider the equation

$$\frac{du^\varepsilon(t)}{dt} = \mathcal{F}(t/\varepsilon, u^\varepsilon(t)), \quad u^\varepsilon(0) = u_0, \tag{7}$$

for a given u_0 and a given periodic function $\mathcal{F}$ (of period P w.r.t. its first variable) which possibly involves stochastic terms. Solution u^ε exhibits high-oscillations in time superimposed to a slow dynamics. Asymptotic techniques -resorting in the present context to *averaging* theory [45]- allow to decompose

$$u^\varepsilon(t) = \Phi_{t/\varepsilon} \circ \Psi_t \circ \Phi_0^{-1}(u_0), \tag{8}$$

into a fast solution component, the εP-periodic change of variable $\Phi_{t/\varepsilon}$, and a slow component, the flow Ψ_t of a non-stiff *averaged* differential equation. Although equation (5) can be satisfied only up to a small remainder, various methods have been recently introduced in situations where (4) is posed in $\mathbb{R}^n$ or for the Schrödinger equation (1).

In the asymptotic behavior $\varepsilon \to 0$, it can be advantageous to replace the original singularly perturbed model (for instance (1) or (2)) by an approximate model which does not contain stiffness any longer. Such reduced models can be derived using asymptotic analysis, namely averaging methods in the case of highly-oscillatory problems. In this project, we also plan to go beyond the mere derivation of limit models, by searching for better approximations of the original problem. This step is of mathematical interest *per se* but it also paves the way of the construction of multiscale numerical methods.

3.1.2.1. Asymptotic analysis of highly-oscillatory PDEs (All members)

Derivation of asymptotic problems

We intend to study the asymptotic behavior of highly-oscillatory evolution equations of the form (4) posed in an infinite dimensional Banach space.

Recently, the stroboscopic averaging has been extended to the PDE context, considering nonlinear Schrödinger equation (1) in the highly-oscillatory regime. A very exciting way would be to use this averaging strategy for highly-oscillatory kinetic problem (2) as those encountered in strongly magnetized plasmas. This turns out to be a very promising way to re-derive gyrokinetic models which are the basis of tokamak simulations in the physicists community. In contract with models derived in the literature (see [34]) which only capture the average with respect to the oscillations, this strategy allows for the complete recovery of the exact solution from the asymptotic (non stiff) model. This can be done by solving companion transport equation that stems naturally from the decomposition (5).

Long-time behavior of Hamiltonian systems
The study of long-time behavior of nonlinear Hamiltonian systems have received a lot of interest during the last decades. It enables to put in light some characteristic phenomena in complex situations, which are beyond the reach of numerical simulations. This kind of analysis is of great interest since it can provide very precise properties of the solution. In particular, we will focus on the dynamics of nonlinear PDEs when the initial condition is close to a stationary solution. Then, the long-time behavior of the solution is studied through mainly three axis

- *linear stability*: considering the linearized PDE, do we have stability of a stationary solution ? Do we have linear Landau damping around stable non homogeneous stationary states?
- *nonlinear stability*: under a criteria, do we have stability of a stationary solution in energy norm like in [42], and does this stability persist under numerical discretization? For example one of our goals is to address the question of the existence and stability of discrete travelling wave in space and time.
- do we have existence of damped solutions for the full nonlinear problem ? Around homogeneous stationary states, solutions scatter towards a modified stationary state (see [43], [39]). The question of existence of Landau damping effects around non homogeneous states is still open and is one of our main goal in the next future.

Asymptotic behavior of stochastic PDEs
The study of SPDEs has known a growing interest recently, in particular with the fields medal of M. Hairer in 2014. In many applications such as radiative transfer, molecular dynamics or simulation of optical fibers, part of the physical interactions are naturally modeled by adding supplementary random terms (the noise) to the initial deterministic equations. From the mathematical point of view, such terms change drastically the behavior of the system.

- In the presence of noise, highly-oscillatory dispersive equations presents new problems. In particular, to study stochastic averaging of the solution, the analysis of the long time behavior of stochastic dispersive equations is required, which is known to be a difficult problem in the general case. In some cases (for instance highly-oscillatory Schrödinger equation (1) with a time white noise in the regime $\varepsilon \ll 1$), it is however possible to perform the analysis and to obtain averaged stochastic equations. We plan to go further by considering more difficult problems, such as the convergence of a stochastic Klein-Gordon-Zakharov system to as stochastic nonlinear Schrödinger equation.
- The long-time behavior of stochastic Schrödinger equations is of great interest to analyze mathematically the validity of the Zakharov theory for wave turbulence (see [44]). The problem of wave turbulence can be viewed either as a deterministic Hamiltonian PDE with random initial data or a randomly forced PDEs where the stochastic forcing is concentrated in some part of the spectrum (in this sense it is expected to be a hypoelliptic problem). One of our goals is to test the validity the Zakharov equation, or at least to make rigorous the spectrum distribution spreading observed in the numerical experiments.

3.1.2.2. Numerical schemes for highly-oscillatory problems (All members)

This section proposes to explore numerical issues raised by highly-oscillatory nonlinear PDEs for which (4) is a prototype. Simulating a highly-oscillatory phenomenon usually requires to adapt the numerical parameters in order to solve the period of size ε so as to accurately simulate the solution over each period, resulting in a unacceptable execution cost. Then, it is highly desirable to derive numerical schemes able to advance the solution by a time step independent of ε. To do so, our goal is to construct *Uniformly Accurate* (UA) numerical schemes, for which the numerical error can be estimated by Ch^p (h being any numerical parameters) with C independent of ε and p the order of the numerical scheme.

Recently, such numerical methods have been proposed by members of the team in the highly-oscillatory context [36]. They are mainly based on a separation of the fast and slow variables, as suggested by the decomposition (5). An additional ingredient to prove the uniformly accuracy of the method for (4) relies on the search for an appropriate initial data which enables to make the problem smooth with respect to ε.

Such an approach is assuredly powerful since it provides a numerical method which enables to capture the high oscillations in time of the solution (and not only its average) even with a large time step. Moreover, in the asymptotic regime, the potential gain is of order $1/\varepsilon$ in comparison with standard methods, and finally averaged models are not able to capture the intermediate regime since they miss important information of the original problem. We are strongly convinced that this strategy should be further studied and extended to cope with some other problems. The ultimate goal being to construct a scheme for the original equation which degenerates automatically into a consistent approximation of the averaged model, without resolving it, the latter can be very difficult to solve.

- Space oscillations:
  When rapidly oscillating coefficients in **space** (*i.e.* terms of the form $a(x, x/\varepsilon)$) occur in elliptic or parabolic equations, homogenization theory and numerical homogenization are usually employed to handle the stiffness. However, these strategies are in general not accurate for all $\varepsilon \in]0, 1]$. Then, the construction of numerical schemes which are able to handle both regimes in an uniform way is of great interest. Separating fast and slow *spatial* scales merits to be explored in this context. The delicate issue is then to extend the choice suitable initial condition to an *appropriate choice of boundary conditions* of the augmented problem.
- Space-time oscillations:
  For more complex problems however, the recent proposed approaches fail since the main oscillations cannot be identified explicitly. This is the case for instance when the magnetic field B depends on t or x in (2) but also for many other physical problems. We then have to deal with the delicate issue of space-time oscillations, which is known to be a very difficult problem from a mathematical and a numerical point of view. To take into account the space-time mixing, a periodic motion has to be detected together with a phase S which possibly depends on the time and space variables. These techniques originate from **geometric optics** which is a very popular technique to handle highly-frequency waves.
- Geometrical properties:
  The questions related to the geometric aspects of multiscale numerical schemes are of crucial importance, in particular when long-time simulations are addressed (see [40]). Indeed, one of the main questions of geometric integration is whether intrinsic properties of the solution may be passed onto its numerical approximation. For instance, if the model under study is Hamiltonian, then the exact flow is symplectic, which motivates the design of symplectic numerical approximation. For practical simulations of Hamiltonian systems, symplectic methods are known to possess very nice properties (see [40]). It is important to combine multiscale techniques to geometric numerical integration. All the problems and equations we intend to deal with will be addressed with a view to preserve intrinsic geometric properties of the exact solutions and/or to approach the asymptotic limit of the system in presence of a small parameter. An example of a numerical method developed by members of the team is the multi-revolution method.
- Quasi-periodic case:

So far, numerical methods have been proposed for the periodic case with single frequency. However, the quasi-periodic case [0] is still misunderstood although many complex problems involve multi-frequencies. Even if the quasi-periodic averaging is doable from a theoretical point of view in the ODE case (see [45]), it is unclear how it can be extended to PDEs. One of the main obstacle being the requirement, usual for ODEs like (4), for $\mathcal{F}$ to be analytic in the periodic variables, an assumption which is clearly impossible to meet in the PDE setting. An even more challenging problem is then the design of numerical methods for this problem.

- extension to stochastic PDEs:
  All these questions will be revisited within the stochastic context. The mathematical study opens the way to the derivation of efficient multiscale numerical schemes for this kind of problems. We believe that the theory is now sufficiently well understood to address the derivation and numerical analysis of multiscale numerical schemes. Multi-revolution composition methods have been recently extended to highly-oscillatory stochastic differential equations The generalization of such multiscale numerical methods to SPDEs is of great interest. The analysis and simulation of numerical schemes for highly-oscillatory nonlinear stochastic Schrödinger equation under diffusion-approximation for instance will be one important objective for us. Finally, an important aspect concerns the quantification of uncertainties in highly-oscillatory kinetic or quantum models (due to an incomplete knowledge of coefficients or imprecise measurement of datas). The construction of efficient multiscale numerical methods which can handle multiple scales as well as random inputs have important engineering applications (see (4.1)).

[0] replacing t/ε by $t\omega/\varepsilon$ in (4), with $\omega \in \mathbb{R}^d$ a vector of non-resonant frequencies

MOKAPLAN Project-Team

3. Research Program

3.1. Modeling and Analysis

The first layer of methodological tools developed by our team is a set of theoretical continuous models that aim at formalizing the problems studied in the applications. These theoretical findings will also pave the way to efficient numerical solvers that are detailed in Section 3.2 .

3.1.1. Static Optimal Transport and Generalizations

3.1.1.1. Convexity constraint and Principal Agent problem in Economics.

(*Participants:* G. Carlier, J-D. Benamou, V. Duval, Xavier Dupuis (LUISS Guido Carli University, Roma)) The principal agent problem plays a distinguished role in the literature on asymmetric information and contract theory (with important contributions from several Nobel prizes such as Mirrlees, Myerson or Spence) and it has many important applications in optimal taxation, insurance, nonlinear pricing. The typical problem consists in finding a cost minimizing strategy for a monopolist facing a population of agents who have an unobservable characteristic, the principal therefore has to take into account the so-called incentive compatibilty constraint which is very similar to the cyclical monotonicity condition which characterizes optimal transport plans. In a special case, Rochet and Choné [156] reformulated the problem as a variational problem subject to a convexity constraint. For more general models, and using ideas from Optimal Transportation, Carlier [90] considered the more general c-convexity constraint and proved a general existence result. Using the formulation of [90] McCann, Figalli and Kim [114] gave conditions under which the principal agent problem can be written as an infinite dimensional convex variational problem. The important results of [114] are intimately connected to the regularity theory for optimal transport and showed that there is some hope to numerically solve the principal-agent problem for general utility functions.
Our expertise: We have already contributed to the numerical resolution of the Principal Agent problem in the case of the convexity constraint, see [95], [146], [143].
Goals: So far, the mathematical PA model can be numerically solved for simple utility functions. A Bregman approach inspired by [54] is currently being developed [93] for more general functions. It would be extremely useful as a complement to the theoretical analysis. A new semi-Discrete Geometric approach is also investigated where the method reduces to non-convex polynomial optimization.

3.1.1.2. Optimal transport and conditional constraints in statistics and finance.

(*Participants:* G. Carlier, J-D. Benamou, G. Peyré) A challenging branch of emerging generalizations of Optimal Transportation arising in *economics, statistics and finance* concerns Optimal Transportation with *conditional* constraints. The *martingale optimal transport* [48], [119] which appears naturally in mathematical finance aims at computing robust bounds on option prices as the value of an optimal transport problem where not only the marginals are fixed but the coupling should be the law of a martingale, since it represents the prices of the underlying asset under the risk-neutral probability at the different dates. Note that as soon as more than two dates are involved, we are facing a multimarginal problem.
Our expertise: Our team has a deep expertise on the topic of OT and its generalization, including many already existing collaboration between its members, see for instance [54], [60], [52] for some representative recent collaborative publications.
Goals: This is a non trivial extension of Optimal Transportation theory and MOKAPLAN will develop numerical methods (in the spirit of entropic regularization) to address it. A popular problem in statistics is the so-called quantile regression problem, recently Carlier, Chernozhukov and Galichon [91] used an Optimal Transportation approach to extend quantile regression to several dimensions. In this approach again, not only fixed marginals constraints are present but also constraints on conditional means. As in the martingale Optimal Transportation problem, one has to deal with an extra conditional constraint. The duality approach usually breaks down under such constraints and characterization of optimal couplings is a challenging task both from a theoretical and numerical viewpoint.

3.1.1.3. JKO gradient flows.

(*Participants:* G. Carlier, J-D. Benamou, M. Laborde, Q. Mérigot, V. Duval) The connection between the static and dynamic transportation problems (see Section 2.3) opens the door to many extensions, most notably by leveraging the use of gradient flows in metric spaces. The flow with respect to the transportation distance has been introduced by Jordan-Kindelherer-Otto (JKO) [126] and provides a variational formulation of many linear and non-linear diffusion equations. The prototypical example is the Fokker Planck equation. We will explore this formalism to study new variational problems over probability spaces, and also to derive innovative numerical solvers. The JKO scheme has been very successfully used to study evolution equations that have the structure of a gradient flow in the Wasserstein space. Indeed many important PDEs have this structure: the Fokker-Planck equation (as was first considered by [126]), the porous medium equations, the granular media equation, just to give a few examples. It also finds application in image processing [79]. Figure 4 shows examples of gradient flows.
Our expertise: There is an ongoing collaboration between the team members on the theoretical and numerical analysis of gradient flows.
Goals: We apply and extend our research on JKO numerical methods to treat various extensions:

- Wasserstein gradient flows with a non displacement convex energy (as in the parabolic-elliptic Keller-Segel chemotaxis model [97])
- systems of evolution equations which can be written as gradient flows of some energy on a product space (possibly mixing the Wasserstein and L^2 structures) : multi-species models or the parabolic-parabolic Keller-Segel model [64]
- perturbation of gradient flows: multi-species or kinetic models are not gradient flows, but may be viewed as a perturbation of Wasserstein gradient flows, we shall therefore investigate convergence of splitting methods for such equations or systems.

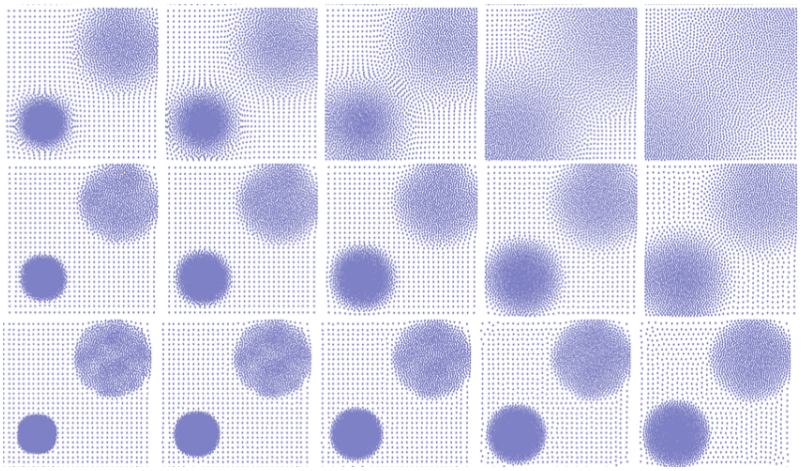

Figure 4. Example of non-linear diffusion equations solved with a JKO flow [56]. The horizontal axis shows the time evolution minimizing the functional $\int \frac{\rho^\alpha}{\alpha-1}$ on the density ρ (discretized here using point clouds, i.e. sum of Diracs' with equal mass). Each row shows a different value of $\alpha = (0.6, 2, 3)$

3.1.1.4. From networks to continuum congestion models.

(*Participants:* G. Carlier, J-D. Benamou, G. Peyré) Congested transport theory in the discrete framework of networks has received a lot of attention since the 50's starting with the seminal work of Wardrop. A few years later, Beckmann proved that equilibria are characterized as solution of a convex minimization problem. However, this minimization problem involves one flow variable per path on the network, its dimension thus quickly becomes too large in practice. An alternative, is to consider continuous in space models of congested optimal transport as was done in [94] which leads to very degenerate PDEs [70].
Our expertise: MOKAPLAN members have contributed a lot to the analysis of congested transport problems and to optimization problems with respect to a metric which can be attacked numerically by fast marching methods [60].
Goals: The case of general networks/anisotropies is still not well understood, general Γ-convergence results will be investigated as well as a detailed analysis of the corresponding PDEs and numerical methods to solve them. Benamou and Carlier already studied numerically some of these PDEs by an augmented Lagrangian method see figure 5 . Note that these class of problems share important similarities with metric learning problem in machine learning, detailed below.

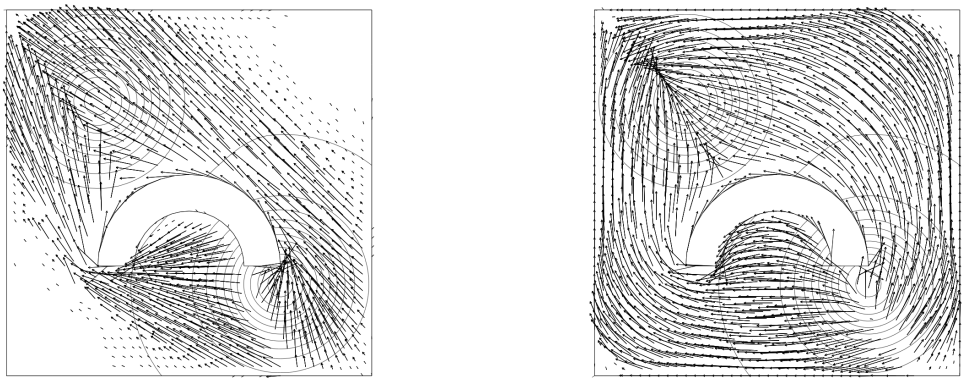

Figure 5. Monge and Wardrop flows of mass around an obstacle [52]. the source/target mass is represented by the level curves. Left : no congestion, Right : congestion.

3.1.2. Diffeomorphisms and Dynamical Transport

3.1.2.1. Growth Models for Dynamical Optimal Transport.

(*Participants:* F-X. Vialard, J-D. Benamou, G. Peyré, L. Chizat) A major issue with the standard dynamical formulation of OT is that it does not allow for variation of mass during the evolution, which is required when tackling medical imaging applications such as tumor growth modeling [82] or tracking elastic organ movements [160]. Previous attempts [137], [153] to introduce a source term in the evolution typically lead to mass teleportation (propagation of mass with infinite speed), which is not always satisfactory.
Our expertise: Our team has already established key contributions both to connect OT to fluid dynamics [50] and to define geodesic metrics on the space of shapes and diffeomorphisms [102].
Goals: Lenaic Chizat's PhD thesis aims at bridging the gap between dynamical OT formulation, and LDDDM diffeomorphisms models (see Section 2.3). This will lead to biologically-plausible evolution models that are both more tractable numerically than LDDM competitors, and benefit from strong theoretical guarantees associated to properties of OT.

3.1.2.2. Mean-field games.

(*Participants:* G. Carlier, J-D. Benamou) The Optimal Transportation Computational Fluid Dynamics (CFD) formulation is a limit case of variational Mean-Field Games (MFGs), a new branch of game theory recently developed by J-M. Lasry and P-L. Lions [130] with an extremely wide range of potential applications [122]. Non-smooth proximal optimization methods used successfully for the Optimal Transportation can be used in the case of deterministic MFGs with singular data and/or potentials [53]. They provide a robust treatment of the positivity constraint on the density of players.
Our expertise: J.-D. Benamou has pioneered with Brenier the CFD approach to Optimal Transportation. Regarding MFGs, on the numerical side, our team has already worked on the use of augmented Lagrangian methods in MFGs [52] and on the analytical side [89] has explored rigorously the optimality system for a singular CFD problem similar to the MFG system.
Goals: We will work on the extension to stochastic MFGs. It leads to non-trivial numerical difficulties already pointed out in [41].

3.1.2.3. Macroscopic Crowd motion, congestion and equilibria.

(*Participants:* G. Carlier, J-D. Benamou, Q. Mérigot, F. Santambrogio (U. Paris-Sud), Y. Achdou (Univ. Paris 7), R. Andreev (Univ. Paris 7)) Many models from PDEs and fluid mechanics have been used to give a description of *people or vehicles moving in a congested environment*. These models have to be classified according to the dimension (1D model are mostly used for cars on traffic networks, while 2-D models are most suitable for pedestrians), to the congestion effects ("soft" congestion standing for the phenomenon where high densities slow down the movement, "hard" congestion for the sudden effects when contacts occur, or a certain threshold is attained), and to the possible rationality of the agents Maury et al [141] recently developed a theory for 2D hard congestion models without rationality, first in a discrete and then in a continuous framework. This model produces a PDE that is difficult to attack with usual PDE methods, but has been successfully studied via Optimal Transportation techniques again related to the JKO gradient flow paradigm. Another possibility to model crowd motion is to use the mean field game approach of Lions and Lasry which limits of Nash equilibria when the number of players is large. This also gives macroscopic models where congestion may appear but this time a global equilibrium strategy is modelled rather than local optimisation by players like in the JKO approach. Numerical methods are starting to be available, see for instance [41], [78].
Our expertise: We have developed numerical methods to tackle both the JKO approach and the MFG approach. The Augmented Lagrangian (proximal) numerical method can actually be applied to both models [52], JKO and deterministic MFGs.
Goals: We want to extend our numerical approach to more realistic congestion model where the speed of agents depends on the density, see Figure 6 for preliminary results. Comparison with different numerical approaches will also be performed inside the ANR ISOTACE. Extension of the Augmented Lagrangian approach to Stochastic MFG will be studied.

3.1.2.4. Diffeomorphic image matching.

(*Participants:* F-X. Vialard, G. Peyré, B. Schmitzer, L. Chizat) Diffeomorphic image registration is widely used in medical image analysis. This class of problems can be seen as the computation of a generalized optimal transport, where the optimal path is a geodesic on a group of diffeomorphisms. The major difference between the two approaches being that optimal transport leads to non smooth optimal maps in general, which is however compulsory in diffeomorphic image matching. In contrast, optimal transport enjoys a convex variational formulation whereas in LDDMM the minimization problem is non convex.
Our expertise: F-X. Vialard is an expert of diffeomorphic image matching (LDDMM) [165], [76], [163]. Our team has already studied flows and geodesics over non-Riemannian shape spaces, which allows for piecewise smooth deformations [102].

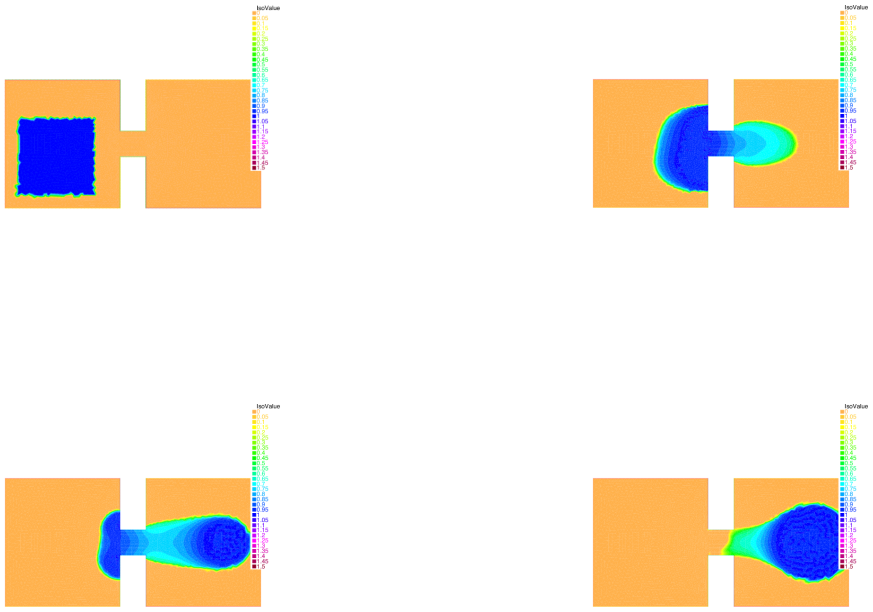

Figure 6. Example of crowd congestion with density dependent speed. The macroscopic density, at 4 different times, of people forced to exit from one room towards a meeting point in a second room.

Goals: Our aim consists in bridging the gap between standard optimal transport and diffeomorphic methods by building new diffeomorphic matching variational formulations that are convex (geometric obstructions might however appear). A related perspective is the development of new registration/transport models in a Lagrangian framework, in the spirit of [159], [160] to obtain more meaningful statistics on longitudinal studies.

Diffeomorphic matching consists in the minimization of a functional that is a sum of a deformation cost and a similarity measure. The choice of the similarity measure is as important as the deformation cost. It is often chosen as a norm on a Hilbert space such as functions, currents or varifolds. From a Bayesian perspective, these similarity measures are related to the noise model on the observed data which is of geometric nature and it is not taken into account when using Hilbert norms. Optimal transport fidelity have been used in the context of signal and image denoising [132], and it is an important question to extends these approach to registration problems. Therefore, we propose to develop similarity measures that are geometric and computationally very efficient using entropic regularization of optimal transport.

Our approach is to use a regularized optimal transport to design new similarity measures on all of those Hilbert spaces. Understanding the precise connections between the evolution of shapes and probability distributions will be investigated to cross-fertilize both fields by developing novel transportation metrics and diffeomorphic shape flows.

The corresponding numerical schemes are however computationally very costly. Leveraging our understanding of the dynamic optimal transport problem and its numerical resolution, we propose to develop new algorithms. These algorithms will use the smoothness of the Riemannian metric to improve both accuracy and speed, using for instance higher order minimization algorithm on (infinite dimensional) manifolds.

3.1.2.5. Metric learning and parallel transport for statistical applications.

(*Participants:* F-X. Vialard, G. Peyré, B. Schmitzer, L. Chizat) The LDDMM framework has been advocated to enable statistics on the space of shapes or images that benefit from the estimation of the deformation. The statistical results of it strongly depend on the choice of the Riemannian metric. A possible direction consists in learning the right invariant Riemannian metric as done in [166] where a correlation matrix (Figure 7) is learnt which represents the covariance matrix of the deformation fields for a given population of shapes. In the same direction, a question of emerging interest in medical imaging is the analysis of time sequence of shapes (called longitudinal analysis) for early diagnosis of disease, for instance [115]. A key question is the inter subject comparison of the organ evolution which is usually done by transport of the time evolution in a common coordinate system via parallel transport or other more basic methods. Once again, the statistical results (Figure 8) strongly depend on the choice of the metric or more generally on the connection that defines parallel transport.
Our expertise: Our team has already studied statistics on longitudinal evolutions in [115], [116].
Goals: Developing higher order numerical schemes for parallel transport (only low order schemes are available at the moment) and developing variational models to learn the metric or the connections for improving statistical results.

3.1.3. Sparsity in Imaging

3.1.3.1. Inverse problems over measures spaces.

(*Participants:* G. Peyré, V. Duval, C. Poon, Q. Denoyelle) As detailed in Section 2.4 , popular methods for regularizing inverse problems in imaging make use of variational analysis over infinite-dimensional (typically non-reflexive) Banach spaces, such as Radon measures or bounded variation functions.
Our expertise: We have recently shown in [164] how – in the finite dimensional case – the non-smoothness of the functionals at stake is crucial to enforce the emergence of geometrical structures (edges in images or fractures in physical materials [65]) for discrete (finite dimensional) problems. We extended this result in a simple infinite dimensional setting, namely sparse regularization of Radon measures for deconvolution [110]. A deep understanding of those continuous inverse problems is crucial to analyze the behavior of their discrete counterparts, and in [111] we have taken advantage of this understanding to develop a fine analysis of the artifacts induced by discrete (*i.e.* which involve grids) deconvolution models. These works are also closely

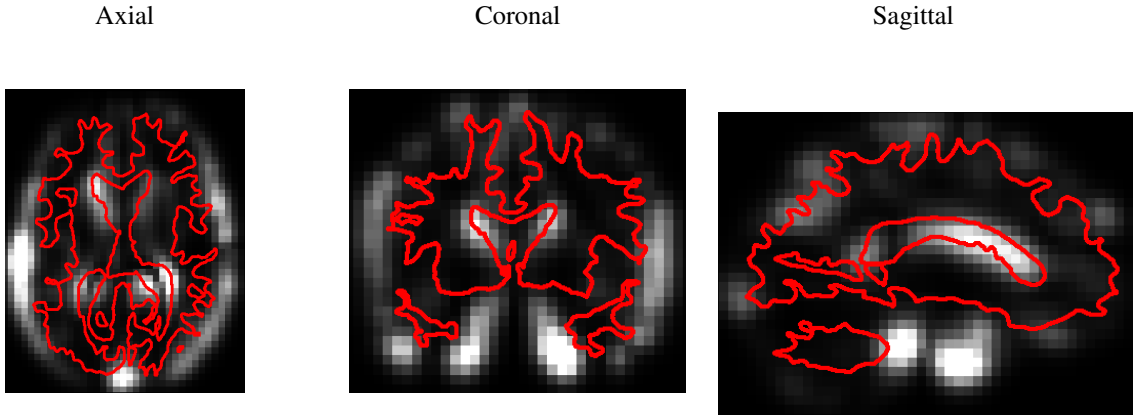

Figure 7. Learning Riemannian metrics in diffeomorphic image matching to capture the brain variability: a diagonal operator that encodes the Riemannian metric is learnt on a template brain out of a collection of brain images. The values of the diagonal operator are shown in greyscale. The red curves represent the boundary between white and grey matter. For more details, we refer the reader to [166], which was a first step towards designing effective and robust metric learning algorithms.

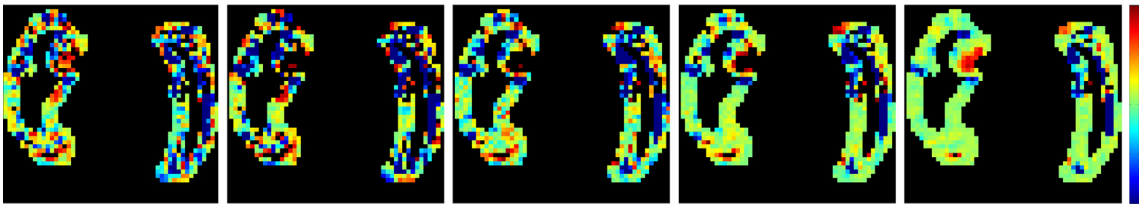

Figure 8. Statistics on initial momenta: In [115], we compared several intersubject transport methodologies to perform statistics on longitudinal evolutions. These longitudinal evolutions are represented by an initial velocity field on the shapes boundaries and these velocity fields are then compared using logistic regression methods that are regularized. The four pictures represent different regularization methods such as L^2, H^1 and regularization including a sparsity prior such as Lasso, Fused Lasso and TV.

related to the problem of limit analysis and yield design in mechanical plasticity, see [92], [65] for an existing collaboration between MOKAPLAN's team members.
Goals: A current major front of research in the mathematical analysis of inverse problems is to extend these results for more complicated infinite dimensional signal and image models, such as for instance the set of piecewise regular functions. The key bottleneck is that, contrary to sparse measures (which are finite sums of Dirac masses), here the objects to recover (smooth edge curves) are not parameterized by a finite number of degrees of freedom. The relevant previous work in this direction are the fundamental results of Chambolle, Caselles and co-workers [49], [43], [98]. They however only deal with the specific case where there is no degradation operator and no noise in the observations. We believe that adapting these approaches using our construction of vanishing derivative pre-certificate [110] could lead to a solution to these theoretical questions.

3.1.3.2. Sub-Riemannian diffusions.

(*Participants:* G. Peyré, J-M. Mirebeau, D. Prandi) Modeling and processing natural images require to take into account their geometry through anisotropic diffusion operators, in order to denoise and enhance directional features such as edges and textures [152], [112]. This requirement is also at the heart of recently proposed models of cortical processing [151]. A mathematical model for these processing is diffusion on sub-Riemanian manifold. These methods assume a fixed, usually linear, mapping from the 2-D image to a lifted function defined on the product of space and orientation (which in turn is equipped with a sub-Riemannian manifold structure).
Our expertise: J-M. Mirebeau is an expert in the discretization of highly anisotropic diffusions through the use of locally adaptive computational stencils [144], [112]. G. Peyré has done several contributions on the definition of geometric wavelets transform and directional texture models, see for instance [152]. Dario Prandi has recently applied methods from sub-Riemannian geometry to image restoration [67].
Goals: A first aspect of this work is to study non-linear, data-adaptive, lifting from the image to the space/orientation domain. This mapping will be implicitly defined as the solution of a convex variational problem. This will open both theoretical questions (existence of a solution and its geometrical properties, when the image to recover is piecewise regular) and numerical ones (how to provide a faithful discretization and fast second order Newton-like solvers). A second aspect of this task is to study the implication of these models for biological vision, in a collaboration with the UNIC Laboratory (directed by Yves Fregnac), located in Gif-sur-Yvette. In particular, the study of the geometry of singular vectors (or "ground states" using the terminology of [61]) of the non-linear sub-Riemannian diffusion operators is highly relevant from a biological modeling point of view.

3.1.3.3. Sparse reconstruction from scanner data.

(*Participants:* G. Peyré, V. Duval, C. Poon) Scanner data acquisition is mathematically modeled as a (sub-sampled) Radon transform [123]. It is a difficult inverse problem because the Radon transform is ill-posed and the set of observations is often aggressively sub-sampled and noisy [158]. Typical approaches [129] try to recover piecewise smooth solutions in order to recover precisely the position of the organ being imaged. There is however a very poor understanding of the actual performance of these methods, and little is known on how to enhance the recovery.
Our expertise: We have obtained a good understanding of the performance of inverse problem regularization on *compact* domains for pointwise sources localization [110].
Goals: We aim at extending the theoretical performance analysis obtained for sparse measures [110] to the set of piecewise regular 2-D and 3-D functions. Some interesting previous work of C. Poon et al [154] (C. Poon is currently a postdoc in MOKAPLAN) have tackled related questions in the field of variable Fourier sampling for compressed sensing application (which is a toy model for fMRI imaging). These approaches are however not directly applicable to Radon sampling, and require some non-trivial adaptations. We also aim at better exploring the connection of these methods with optimal-transport based fidelity terms such as those introduced in [40].

3.1.3.4. Tumor growth modeling in medical image analysis.

(*Participants:* G. Peyré, F-X. Vialard, J-D. Benamou, L. Chizat) Some applications in medical image analysis require to track shapes whose evolution is governed by a growth process. A typical example is tumor growth, where the evolution depends on some typically unknown but meaningful parameters that need to be estimated. There exist well-established mathematical models [82], [150] of non-linear diffusions that take into account recently biologically observed property of tumors. Some related optimal transport models with mass variations have also recently been proposed [139], which are connected to so-called metamorphoses models in the LDDMM framework [62].
Our expertise: Our team has a strong experience on both dynamical optimal transport models and diffeomorphic matching methods (see Section 3.1.2).
Goals: The close connection between tumor growth models [82], [150] and gradient flows for (possibly non-Euclidean) Wasserstein metrics (see Section 3.1.2) makes the application of the numerical methods we develop particularly appealing to tackle large scale forward tumor evolution simulation. A significant departure from the classical OT-based convex models is however required. The final problem we wish to solve is the backward (inverse) problem of estimating tumor parameters from noisy and partial observations. This also requires to set-up a meaningful and robust data fidelity term, which can be for instance a generalized optimal transport metric.

3.2. Numerical Tools

The above continuous models require a careful discretization, so that the fundamental properties of the models are transferred to the discrete setting. Our team aims at developing innovative discretization schemes as well as associated fast numerical solvers, that can deal with the geometric complexity of the variational problems studied in the applications. This will ensure that the discrete solution is correct and converges to the solution of the continuous model within a guaranteed precision. We give below examples for which a careful mathematical analysis of the continuous to discrete model is essential, and where dedicated non-smooth optimization solvers are required.

3.2.1. Geometric Discretization Schemes

3.2.1.1. Discretizing the cone of convex constraints.

(*Participants:* J-D. Benamou, G. Carlier, J-M. Mirebeau, Q. Mérigot) Optimal transportation models as well as continuous models in economics can be formulated as infinite dimensional convex variational problems with the constraint that the solution belongs to the cone of convex functions. Discretizing this constraint is however a tricky problem, and usual finite element discretizations fail to converge.
Our expertise: Our team is currently investigating new discretizations, see in particular the recent proposal [59] for the Monge-Ampère equation and [143] for general non-linear variational problems. Both offer convergence guarantees and are amenable to fast numerical resolution techniques such as Newton solvers. Since [59] explaining how to treat efficiently and in full generality Transport Boundary Conditions for Monge-Ampère, this is a promising fast and new approach to compute Optimal Transportation viscosity solutions. A monotone scheme is needed. One is based on Froese Oberman work [118], a new different and more accurate approach has been proposed by Mirebeau, Benamou and Collino [57]. As shown in [104], discretizing the constraint for a continuous function to be convex is not trivial. Our group has largely contributed to solve this problem with G. Carlier [95], Quentin Mérigot [146] and J-M. Mirebeau [143]. This problem is connected to the construction of monotone schemes for the Monge-Ampère equation.
Goals: The current available methods are 2-D. They need to be optimized and parallelized. A non-trivial extension to 3-D is necessary for many applications. The notion of c-convexity appears in optimal transport for generalized displacement costs. How to construct an adapted discretization with "good" numerical properties is however an open problem.

3.2.1.2. Numerical JKO gradient flows.

(*Participants:* J-D. Benamou, G. Carlier, J-M. Mirebeau, G. Peyré, Q. Mérigot) As detailed in Section 2.3 , gradient Flows for the Wasserstein metric (aka JKO gradient flows [126]) provides a variational formulation of many non-linear diffusion equations. They also open the way to novel discretization schemes. From a computational point, although the JKO scheme is constructive (it is based on the implicit Euler scheme), it has not been very much used in practice numerically because the Wasserstein term is difficult to handle (except in dimension one).
Our expertise:

Solving one step of a JKO gradient flow is similar to solving an Optimal transport problem. A geometrical a discretization of the Monge-Ampère operator approach has been proposed by Mérigot, Carlier, Oudet and Benamou in [56] see Figure 4 . The Gamma convergence of the discretisation (in space) has been proved.
Goals: We are also investigating the application of other numerical approaches to Optimal Transport to JKO gradient flows either based on the CFD formulation or on the entropic regularization of the Monge-Kantorovich problem (see section 3.2.3). An in-depth study and comparison of all these methods will be necessary.

3.2.2. Sparse Discretization and Optimization

3.2.2.1. From discrete to continuous sparse regularization and transport.

(*Participants:* V. Duval, G. Peyré, G. Carlier, Jalal Fadili (ENSICaen), Jérôme Malick (CNRS, Univ. Grenoble)) While pervasive in the numerical analysis community, the problem of discretization and Γ-convergence from discrete to continuous is surprisingly over-looked in imaging sciences. To the best of our knowledge, our recent work [110], [111] is the first to give a rigorous answer to the transition from discrete to continuous in the case of the spike deconvolution problem. Similar problems of Γ-convergence are progressively being investigated in the optimal transport community, see in particular [96].
Our expertise: We have provided the first results on the discrete-to-continous convergence in both sparse regularization variational problems [110], [111] and the static formulation of OT and Wasserstein barycenters [96]
Goals: In a collaboration with Jérôme Malick (Inria Grenoble), our first goal is to generalize the result of [110] to generic partly-smooth convex regularizers routinely used in imaging science and machine learning, a prototypal example being the nuclear norm (see [164] for a review of this class of functionals). Our second goal is to extend the results of [96] to the novel class of entropic discretization schemes we have proposed [54], to lay out the theoretical foundation of these ground-breaking numerical schemes.

3.2.2.2. Polynomial optimization for grid-free regularization.

(*Participants:* G. Peyré, V. Duval, I. Waldspurger) There has been a recent spark of attention of the imaging community on so-called "grid free" methods, where one tries to directly tackle the infinite dimensional recovery problem over the space of measures, see for instance [87], [110]. The general idea is that if the range of the imaging operator is finite dimensional, the associated dual optimization problem is also finite dimensional (for deconvolution, it corresponds to optimization over the set of trigonometric polynomials).
Our expertise: We have provided in [110] a sharp analysis of the support recovery property of this class of methods for the case of sparse spikes deconvolution.
Goals: A key bottleneck of these approaches is that, while being finite dimensional, the dual problem necessitates to handle a constraint of polynomial positivity, which is notoriously difficult to manipulate (except in the very particular case of 1-D problems, which is the one exposed in [87]). A possible, but very costly, methodology is to ressort to Lasserre's SDP representation hierarchy [131]. We will make use of these approaches and study how restricting the level of the hierarchy (to obtain fast algorithms) impacts the recovery performances (since this corresponds to only computing approximate solutions). We will pay a particular attention to the recovery of 2-D piecewise constant functions (the so-called total variation of functions regularization [157]), see Figure 3 for some illustrative applications of this method.

3.2.3. First Order Proximal Schemes

3.2.3.1. L^2 proximal methods.

(*Participants:* G. Peyré, J-D. Benamou, G. Carlier, Jalal Fadili (ENSICaen)) Both sparse regularization problems in imaging (see Section 2.4) and dynamical optimal transport (see Section 2.3) are instances of large scale, highly structured, non-smooth convex optimization problems. First order proximal splitting optimization algorithms have recently gained lots of interest for these applications because they are the only ones capable of scaling to giga-pixel discretizations of images and volumes and at the same time handling non-smooth objective functions. They have been successfully applied to optimal transport [50], [147], congested optimal transport [81] and to sparse regularizations (see for instance [155] and the references therein).
Our expertise: The pioneering work of our team has shown how these proximal solvers can be used to tackle the dynamical optimal transport problem [50], see also [147]. We have also recently developed new proximal schemes that can cope with non-smooth composite objectives functions [155].
Goals: We aim at extending these solvers to a wider class of variational problems, most notably optimization under divergence constraints [52]. Another subject we are investigating is the extension of these solvers to both non-smooth and non-convex objective functionals, which are mandatory to handle more general transportation problems and novel imaging regularization penalties.

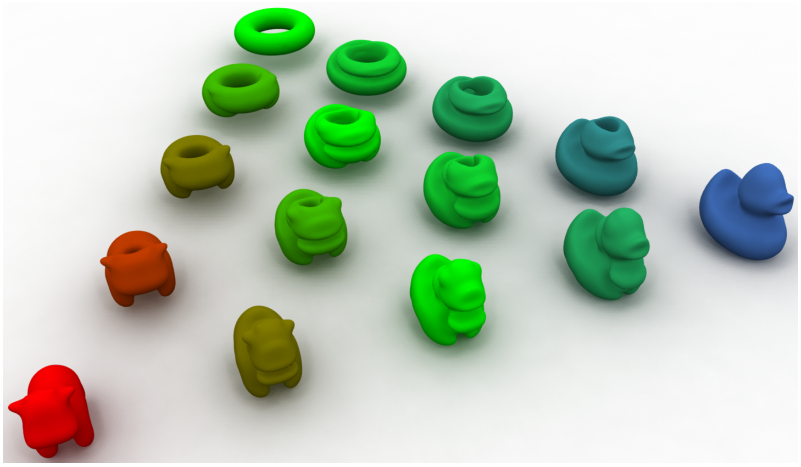

Figure 9. Example of barycenter between shapes computed using optimal transport barycenters of the uniform densities inside the 3 extremal shapes, computed as detailed in [161]. Note that the barycenters are not in general uniform distributions, and we display them as the surface defined by a suitable level-set of the density.

3.2.3.2. Bregman proximal methods.

(*Participants:* G. Peyré G. Carlier, L. Nenna, J-D. Benamou, L. Nenna, Marco Cuturi (Kyoto Univ.)) The entropic regularization of the Kantorovich linear program for OT has been shown to be surprisingly simple and efficient, in particular for applications in machine learning [108]. As shown in [54], this is a special instance of the general method of Bregman iterations, which is also a particular instance of first order proximal schemes according to the Kullback-Leibler divergence.

Our expertise: We have recently [54] shown how Bregman projections [71] and Dykstra algorithm [46] offer a generic optimization framework to solve a variety of generalized OT problems. Carlier and Dupuis [93] have designed a new method based on alternate Dykstra projections and applied it to the *principal-agent problem* in microeconomics. We have applied this method in computer graphics in a paper accepted in SIGGRAPH 2015 [161]. Figure 9 shows the potential of our approach to handle giga-voxel datasets: the input volumetric densities are discretized on a 100^3 computational grid.
Goals: Following some recent works (see in particular [101]) we first aim at studying primal-dual optimization schemes according to Bregman divergences (that would go much beyond gradient descent and iterative projections), in order to offer a versatile and very effective framework to solve variational problems involving OT terms. We then also aim at extending the scope of usage of this method to applications in quantum mechanics (Density Functional Theory, see [105]) and fluid dynamics (Brenier's weak solutions of the incompressible Euler equation, see [72]). The computational challenge is that realistic physical examples are of a huge size not only because of the space discretization of one marginal but also because of the large number of marginals involved (for incompressible Euler the number of marginals equals the number of time steps).

NACHOS Project-Team

3. Research Program

3.1. Scientific foundations

The research activities undertaken by the team aim at developing innovative numerical methodologies putting the emphasis on several features:

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

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

3.2. High order discretization methods

3.2.1. The Discontinuous Galerkin method

The Discontinuous Galerkin method (DG) was introduced in 1973 by Reed and Hill to solve the neutron transport equation. From this time to the 90's a review on the DG methods would likely fit into one page. In the meantime, the Finite Volume approach (FV) has been widely adopted by computational fluid dynamics scientists and has now nearly supplanted classical finite difference and finite element methods in solving problems of non-linear convection and conservation law systems. The success of the FV method is due to its ability to capture discontinuous solutions which may occur when solving non-linear equations or more simply, when convecting discontinuous initial data in the linear case. Let us first remark that DG methods share with FV methods this property since a first order FV scheme may be viewed as a 0th order DG scheme. However a DG method may also be considered as a Finite Element (FE) one where the continuity constraint at an element interface is released. While keeping almost all the advantages of the FE method (large spectrum of applications, complex geometries, etc.), the DG method has other nice properties which explain the renewed interest it gains in various domains in scientific computing as witnessed by books or special issues of journals dedicated to this method [34]- [35]- [36]- [41]:

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

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

3.2.2. High order DG methods for wave propagation models

DG methods are at the heart of the activities of the team regarding the development of high order discretization schemes for the PDE systems modeling electromagnetic and elatsodynamic wave propagation.

- **Nodal DG methods for time-domain problems**. For the numerical solution of the time-domain Maxwell equations, we have first proposed a non-dissipative high order DGTD (Discontinuous Galerkin Time-Domain) method working on unstructured conforming simplicial meshes [9]. This DG method combines a central numerical flux function for the approximation of the integral term at the interface of two neighboring elements with a second order leap-frog time integration scheme. Moreover, the local approximation of the electromagnetic field relies on a nodal (Lagrange type) polynomial interpolation method. Recent achievements by the team deal with the extension of these methods towards non-conforming unstructured [6]-[7] and hybrid structured/unstructured meshes [4], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [3]-[13]-[12]. A high order DG method has also been proposed for the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [2].
- **Hybridizable DG (HDG) method for time-domain and time-harmonic problems**. For the numerical treatment of the time-harmonic Maxwell equations, nodal DG methods can also be considered [5]. 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.*[39] 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[11].
- **Multiscale DG methods for time-domain problems**. More recently, in collaboration with LNCC in Petropolis (Frédéric Valentin) the framework of the HOMAR assoacite team, we are investigating a family of methods specifically designed for an accurate and efficient numerical treatment of multiscale wave propagation problems. These methods, referred to as Multiscale Hybrid Mixed (MHM) methods, are currently studied in the team for both time-domain electromagnetic and elastodynamic PDE models. They consist in reformulating the mixed variational form of each system into a global (arbitrarily coarse) problem related to a weak formulation of the boundary condition (carried by a Lagrange multiplier that represents e.g. the normal stress tensor in elastodynamic sytems), and a series of small, element-wise, fully decoupled problems resembling to the initial one and related to some well chosen partition of the solution variables on each element. By construction, that methodology is fully parallelizable and recursivity may be used in each local problem as well, making MHM methods belonging to multi-level highly parallelizable methods. Each local problem may be solved using DG or classical Galerkin FE approximations combined with some appropriate time integration scheme (θ-scheme or leap-frog scheme).

3.3. Efficient time integration strategies

The use of unstructured meshes (based on triangles in two space dimensions and tetrahedra in three space dimensions) is an important feature of the DGTD methods developed in the team which can thus easily deal with complex geometries and heterogeneous propagation media. Moreover, DG discretization methods are naturally adapted to local, conforming as well as non-conforming, refinement of the underlying mesh. Most of the existing DGTD methods rely on explicit time integration schemes and lead to block diagonal mass matrices which is often recognized as one of the main advantages with regards to continuous finite element methods.

However, explicit DGTD methods are also constrained by a stability condition that can be very restrictive on highly refined meshes and when the local approximation relies on high order polynomial interpolation. There are basically three strategies that can be considered to cure this computational efficiency problem. The first approach is to use an unconditionally stable implicit time integration scheme to overcome the restrictive constraint on the time step for locally refined meshes. In a second approach, a local time stepping strategy is combined with an explicit time integration scheme. In the third approach, the time step size restriction is overcome by using a hybrid explicit-implicit procedure. In this case, one blends a time implicit and a time explicit schemes where only the solution variables defined on the smallest elements are treated implicitly. The first and third options are considered in the team in the framework of DG [3]-[13]-[12] and HDG discretization methods.

3.4. Numerical treatment of complex material models

Towards the general aim of being able to consider concrete physical situations, we are interested in taking into account in the numerical methodologies that we study, a better description of the propagation of waves in realistic media. In the case of electromagnetics, a typical physical phenomenon that one has to consider is *dispersion*. It is present in almost all media and expresses the way the material reacts to an electromagnetic field. In the presence of an electric field a medium does not react instantaneously and thus presents an electric polarization of the molecules or electrons that itself influences the electric displacement. In the case of a linear homogeneous isotropic media, there is a linear relation between the applied electric field and the polarization. However, above some range of frequencies (depending on the considered material), the dispersion phenomenon cannot be neglected and the relation between the polarization and the applied electric field becomes complex. This is rendered via a frequency-dependent complex permittivity. Several models of complex permittivity exist. Concerning biological media, the Debye model is commonly adopted in the presence of water, biological tissues and polymers, so that it already covers a wide range of applications [10]. In the context of nanoplasmonics, one is interested in modeling the dispersion effects on metals on the nanometer scale and at optical frequencies. In this case, the Drude or the Drude-Lorentz models are generally chosen [15]. In the context of seismic wave propagation, we are interested by the intrinsic attenuation of the medium [14]. In realistic configurations, for instance in sedimentary basins where the waves are trapped, we can observe site effects due to local geological and geotechnical conditions which result in a strong increase in amplification and duration of the ground motion at some particular locations. During the wave propagation in such media, a part of the seismic energy is dissipated because of anelastic losses relied to the internal friction of the medium. For these reasons, numerical simulations based on the basic assumption of linear elasticity are no more valid since this assumption results in a severe overestimation of amplitude and duration of the ground motion, even when we are not in presence of a site effect, since intrinsic attenuation is not taken into account.

3.5. High performance numerical computing

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

NANO-D Project-Team

3. Research Program

3.1. The need for practical design of nanosystems

Computing has long been an essential tool of engineering. During the twentieth century, the development of macroscopic engineering has been largely stimulated by progress in numerical design and prototyping. Cars, planes, boats, and many other manufactured objects are nowadays, for the most part, designed and tested on computers. Digital prototypes have progressively replaced actual ones, and effective computer-aided engineering tools (e.g., CATIA, SolidWorks, T-FLEX CAD, Alibre Design, TopSolid, etc.) have helped cut costs and reduce production cycles of macroscopic systems [79].

The twenty-first century is most likely to see a similar development at the atomic scale. Indeed, the recent years have seen tremendous progress in nanotechnology. The magazine Science, for example, recently featured a paper demonstrating an example of DNA nanotechnology, where DNA strands are stacked together through programmable self-assembly [49]. In February 2007, the cover of Nature Nanotechnology showed a "nano-wheel" composed of a few atoms only. Several nanosystems have already been demonstrated, including a *de-novo* computationally designed protein interface [50], a wheelbarrow molecule [60], a nano-car [83], a Morse molecule [33], etc. Typically, these designs are optimized using semi-empirical quantum mechanics calculations, such as the semi-empirical ASED+ calculation technique [34].

While impressive, these are but two examples of the nanoscience revolution already impacting numerous fields, including electronics and semiconductors [64], textiles [63], [54], energy [69], food [44], drug delivery [52], [85], chemicals [55], materials [45], the automotive industry [31], aerospace and defense [51], medical devices and therapeutics [47], medical diagnostics [86], etc. According to some estimates, the world market for nanotechnology-related products and services will reach one trillion dollars by 2015 [78]. Nano-engineering groups are multiplying throughout the world, both in academia and in the industry: in the USA, the MIT has a "NanoEngineering" research group, Sandia National Laboratories created a "National Institute for Nano Engineering", to name a few; China founded a "National Center for Nano Engineering" in 2003, etc. Europe is also a significant force in public funding of nanoscience and nanotechnology and, in Europe, Grenoble and the Rhone-Alpes area gather numerous institutions and organizations related to nanoscience.

Of course, not all small systems that currently fall under the label "nano" have mechanical, electronic, optical properties similar to the examples given above. Furthermore, current construction capabilities lack behind some of the theoretical designs which have been proposed, such as the planetary gear designed by Eric Drexler at Nanorex. However, the trend is clearly for adding more and more functionality to nanosystems. While designing nanosystems is still very much an art mostly performed by physicists, chemists and biologists in labs throughout the world, there is absolutely no doubt that fundamental engineering practices will progressively emerge, and that these practices will be turned into quantitative rules and methods. Similar to what has happened with macroscopic engineering, powerful and generic software will then be employed to engineer complex nanosystems.

3.2. Challenges of practical nanosystem design

As with macrosystems, designing nanosystems will involve modeling and simulation within software applications: modeling, especially structural modeling, will be concerned with the creation of potentially complex chemical structures such as the examples above, using a graphical user interface, parsers, scripts, builders, etc.; simulation will be employed to predict some properties of the constructed models, including mechanical properties, electronic properties, chemical properties, etc.

In general, design may be considered as an "inverse simulation problem". Indeed, designed systems often need to be optimized so that their properties — predicted by simulation — satisfy specific objectives and constraints (e.g. a car should have a low drag coefficient, a drug should have a high affinity and selectivity to a target protein, a nano-wheel should roll when pushed, etc.). Being the main technique employed to predict properties, simulation is essential to the design process. At the nanoscale, simulation is even more important. Indeed, physics significantly constrains atomic structures (e.g. arbitrary inter-atomic distances cannot exist), so that a tentative atomic shape should be checked for plausibility much earlier in the design process (e.g. remove atomic clashes, prevent unrealistic, high-energy configurations, etc.). For nanosystems, thus, efficient simulation algorithms are required both when modeling structures and when predicting systems properties. Precisely, an effective software tool to design nanosystems should (a) allow for interactive physically-based modeling, where all user actions (e.g. displacing atoms, modifying the system's topology, etc.) are automatically followed by a few steps of energy minimization to help the user build plausible structures, even for large number of atoms, and (b) be able to predict systems properties, through a series of increasingly complex simulations.

3.3. Current simulation approaches

Even though the growing need for effective nanosystem design will still increase the demand for simulation, a lot of research has already gone into the development of efficient simulation algorithms. Typically, two approaches are used: (a) increasing the computational resources (use super-computers, computer clusters, grids, develop parallel computing approaches, etc.), or (b) simulating simplified physics and/or models. Even though the first strategy is sometimes favored, it is expensive and, it could be argued, inefficient: only a few supercomputers exist, not everyone is willing to share idle time from their personal computer, etc. Surely, we would see much less creativity in cars, planes, and manufactured objects all around if they had to be designed on one of these scarce super-resources.

The second strategy has received a lot of attention. Typical approaches to speed up molecular mechanics simulation include lattice simulations [89], removing some degrees of freedom (e.g. keeping torsion angles only [62], [84]), coarse-graining [87], [81], [35], [82], multiple time step methods [75], [76], fast multipole methods [48], parallelization [61], averaging [43], multi-scale modeling [42], [39], reactive force fields [41], [92], interactive multiplayer games for predicting protein structures [46], etc. Until recently, quantum mechanics methods, as well as mixed quantum / molecular mechanics methods were still extremely slow. One breakthrough has consisted in the discovery of linear-scaling, divide-and-conquer quantum mechanics methods [90], [91].

Overall, the computational community has already produced a variety of sophisticated simulation packages, for both classical and quantum simulation: ABINIT, AMBER, CHARMM, Desmond, GROMOS and GROMACS, LAMMPS, NAMD, ROSETTA, SIESTA, TINKER, VASP, YASARA, etc. Some of these tools are open source, while some others are available commercially, sometimes via integrating applications: Ascalaph Designer, BOSS, Discovery Studio, Materials Studio, Maestro, MedeA, MOE, NanoEngineer-1, Spartan, etc. Other tools are mostly concerned with visualization, but may sometimes be connected to simulation packages: Avogadro, PyMol, VMD, Zodiac, etc. The nanoHUB network also includes a rich set of tools related to computational nanoscience.

To the best of our knowledge, however, all methods which attempt to speed up dynamics simulations perform a priori simplification assumptions, which might bias the study of the simulated phenomenon. A few recent, interesting approaches have managed to combine several levels of description (e.g. atomistic and coarse-grained) into a single simulation, and have molecules switch between levels during simulation, including the adaptive resolution method [71], [72], [73], [74], the adaptive multiscale method [68], and the adaptive partitioning of the Lagrangian method [56]. Although these approaches have demonstrated some convincing applications, they all suffer from a number of limitations stemming from the fact that they are either ad hoc methods tuned to fix specific problems (e.g. fix density problems in regions where the level of description changes), or mathematically founded methods that necessitate to "calibrate" potentials so that they can be mixed (i.e. all potentials have to agree on a reference point). In general, multi-scale methods, even when

they do not allow molecules to switch between levels of detail during simulation, have to solve the problem of rigorously combining multiple levels of description (i.e. preserve statistics, etc.), of assigning appropriate levels to different parts of the simulated system ("simplify as much as possible, but not too much"), and of determining computable mappings between levels of description (especially, adding back detail when going from coarse-grained descriptions to fine-grained descriptions).

3.4. As-Rigid-As-Possible methods for molecular paths

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

3.5. Modelling and simulation for the characterization of advanced materials

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

RAPSODI Project-Team

3. Research Program

3.1. Design and analysis of structure-preserving schemes

3.1.1. Numerical analysis of nonlinear numerical methods

Up to now, the numerical methods dedicated to degenerate parabolic problems that the mathematicians are able to analyze almost all rely on the use of mathematical transformations (like e.g. the Kirchhoff's transform). It forbids the extension of the analysis to complex realistic models. The methods used in the industrial codes for solving such complex problems rely on the use of what we call NNM, i.e., on methods that preserve all the nonlinearities of the problem without reducing them thanks to artificial mathematical transforms. Our aim is to take advantage of the recent breakthrough proposed by C. Cancès & C. Guichard [69], [4] to develop efficient new numerical methods with a full numerical analysis (stability, convergence, error estimates, robustness w.r.t. physical parameters, ...).

3.1.2. Design and analysis of asymptotic-preserving schemes

There has been an extensive effort in the recent years to develop numerical methods for diffusion equations that are robust with respect to heterogeneities, anisotropy, and the mesh (see for instance [83] for an extensive discussion on such methods). On the other hand, the understanding of the role of nonlinear stability properties in the asymptotic behaviors of dissipative systems increased significantly in the last decades (see for instance [71], [101]).

Recently, C. Chainais-Hillairet and co-authors [64], [72] and [73] developed a strategy based on the control of the numerical counterpart of the physical entropy to develop and analyze AP numerical methods. In particular, these methods show great promises for capturing accurately the behavior of the solutions to dissipative problems when some physical parameter is small with respect to the discretization characteristic parameters, or in the long-time asymptotic. Since it requires the use of nonlinear test functions in the analysis, strong restrictions on the physics (isotropic problems) and on the mesh (Cartesian grids, Voronoï boxes...) are required in [64], [72] and [73]. The schemes proposed in [69] and [4] allow to handle nonlinear test functions in the analysis without restrictions on the mesh and on the anisotropy of the problem. Combining the nonlinear schemes *à la* [69] with the methodology of [64], [72], [73] would provide schemes that are robust both with respect to the meshes and to the parameters. Therefore, they would be also robust under adaptive mesh refinement.

3.1.3. Design and stability analysis of numerical methods for low-Mach models

We aim at extending the range of the `NS2DDV-M` software by introducing new physical models, like for instance the low-Mach model, which gives intermediate solutions between the compressible Navier–Stokes model and the incompressible Navier–Stokes one. This model was introduced in [99] as a limiting system which describes combustion processes at low Mach number in a confined region. Within this scope, we will propose a theoretical study for proving the existence of weak solutions for a particular class of models for which the dynamic viscosity of the fluid is a specific function of the density. We will propose also the extension of a combined Finite Volume-Finite Element method, initially developed for the simulation of incompressible and variable density flows, to this class of models.

3.2. Optimizing the computational efficiency

3.2.1. High-order nonlinear numerical methods

The numerical experiments carried out in [69] show that in case of very strong anisotropy, the convergence of the proposed NNM becomes too slow (less than first order). Indeed, the method appears to strongly overestimate the dissipation. In order to make the method more competitive, it is necessary to estimate the dissipation in a more accurate way. Preliminary numerical results show that second order accuracy in space can be achieved in this way. One also aims to obtain (at least) second order accuracy in time without jeopardizing the stability. For many problems, this can be done by using so-called two-step backward differentiation formulas (BDF2) [87].

Concerning the inhomogeneous fluid models, we aim to investigate new methods for the mass equation resolution. Indeed, we aim at increasing the accuracy while maintaining some positivity-like properties and the efficiency for a wide range of physical parameters. To this end, we will consider Residual Distribution schemes, that appear as an alternative to Finite Volume methods. Residual Distribution schemes enjoy very compact stencils. Therefore, their extension from 2D to 3D yield reasonable difficulties. These methods appeared twenty years ago, but recent extensions to unsteady problems [102], [95], with high-order accuracy [49], [48], or for parabolic problems [46], [47] make them very competitive. Relying on these breakthroughs, we aim at designing new Residual Distribution schemes for fluid mixture models with high-order accuracy while preserving the positivity of the solutions.

3.2.2. A posteriori error control

The question of the *a posteriori* error estimators will also have to be addressed in this optimization context. Since the pioneering papers of Babuska and Rheinboldt more than thirty years ago [54], *a posteriori* error estimators have been widely studied. We will take advantage of the huge corresponding bibliography database in order to optimize our numerical results.

For example, we would like to generalize the results we derived for the harmonic magnetodynamic case (e.g. [74] and [75]) to the temporal magnetodynamic one, for which space/time *a posteriori* error estimators have to be developed. A space/time refinement algorithm should consequently be proposed and tested on academic as well as industrial benchmarks.

We also want to develop *a posteriori* estimators for the variable density Navier–Stokes model or some of its variants. To do so, several difficulties have to be tackled: the problem is nonlinear, unsteady, and the numerical method [66], [67] we developed combines features from Finite Elements and Finite Volumes. Fortunately, we do not start from scratch. Some recent references are devoted to the unsteady Navier–Stokes model in the Finite Element context [61], [105]. In the Finite Volume context, recent references deal with unsteady convection-diffusion equations [104], [52], [81] and [70]. We want to adapt some of these results to the variable density Navier–Stokes system, and to be able to design an efficient space-time remeshing algorithm.

3.2.3. Efficient computation of pairwise interactions in large systems of particles

Many systems are modeled as a large number of punctual individuals (N) which interact pairwise which means $N(N-1)/2$ interactions. Such systems are ubiquitous, they are found in chemistry (Van der Waals interaction between atoms), in astrophysics (gravitational interactions between stars, galaxies or galaxy clusters), in biology (flocking behavior of birds, swarming of fishes) or in the description of crowd motions. Building on the special structure of convolution-type of the interactions, the team develops computation methods based on the Non Uniform Fast Fourier Transform [90]. This reduces the $O(N^2)$ naive computational cost of the interactions to $O(N \log N)$, allowing numerical simulations involving millions of individuals.

CAGE Project-Team

3. Research Program

3.1. Research domain

The activities of CAGE are part of the research in the wide area of control theory. This nowadays mature discipline is still the subject of intensive research because of its crucial role in a vast array of applications.

More specifically, our contributions are in the area of **mathematical control theory**, which is to say that we are interested in the analytical and geometrical aspects of control applications. In this approach, a control system is modeled by a system of equations (of many possible types: ordinary differential equations, partial differential equations, stochastic differential equations, difference equations,...), possibly not explicitly known in all its components, which are studied in order to establish qualitative and quantitative properties concerning the actuation of the system through the control.

Motion planning is, in this respect, a cornerstone property: it denotes the design and validation of algorithms for identifying a control law steering the system from a given initial state to (or close to) a target one. Initial and target positions can be replaced by sets of admissible initial and final states as, for instance, in the motion planning task towards a desired periodic solution. Many specifications can be added to the pure motion planning task, such as robustness to external or endogenous disturbances, obstacle avoidance or penalization criteria. A more abstract notion is that of **controllability**, which denotes the property of a system for which any two states can be connected by a trajectory corresponding to an admissible control law. In mathematical terms, this translates into the surjectivity of the so-called **end-point map**, which associates with a control and an initial state the final point of the corresponding trajectory. The analytical and topological properties of endpoint maps are therefore crucial in analyzing the properties of control systems.

One of the most important additional objective which can be associated with a motion planning task is **optimal control**, which corresponds to the minimization of a cost (or, equivalently, the maximization of a gain) [156]. Optimal control theory is clearly deeply interconnected with calculus of variations, even if the non-interchangeable nature of the time-variable results in some important specific features, such as the occurrence of **abnormal extremals** [119]. Research in optimal control encompasses different aspects, from numerical methods to dynamic programming and non-smooth analysis, from regularity of minimizers to high order optimality conditions and curvature-like invariants.

Another domain of control theory with countless applications is **stabilization**. The goal in this case is to make the system converge towards an equilibrium or some more general safety region. The main difference with respect to motion planning is that here the control law is constructed in feedback form. One of the most important properties in this context is that of **robustness**, i.e., the performance of the stabilization protocol in presence of disturbances or modeling uncertainties. A powerful framework which has been developed to take into account uncertainties and exogenous non-autonomous disturbances is that of hybrid and switched systems [159], [118], [147]. The central tool in the stability analysis of control systems is that of **control Lyapunov function**. Other relevant techniques are based on algebraic criteria or dynamical systems. One of the most important stability property which is studied in the context of control system is **input-to-state stability** [143], which measures how sensitive the system is to an external excitation.

One of the areas where control applications have nowadays the most impressive developments is in the field of **biomedicine and neurosciences**. Improvements both in modeling and in the capability of finely actuating biological systems have concurred in increasing the popularity of these subjects. Notable advances concern, in particular, identification and control for biochemical networks [137] and models for neural activity [105]. Therapy analysis from the point of view of optimal control has also attracted a great attention [140].

Biological models are not the only one in which stochastic processes play an important role. Stock-markets and energy grids are two major examples where optimal control techniques are applied in the non-deterministic setting. Sophisticated mathematical tools have been developed since several decades to allow for such extensions. Many theoretical advances have also been required for dealing with complex systems whose description is based on **distributed parameters** representation and **partial differential equations**. Functional analysis, in particular, is a crucial tool to tackle the control of such systems [153].

Let us conclude this section by mentioning another challenging application domain for control theory: the decision by the European Union to fund a flagship devoted to the development of quantum technologies is a symptom of the role that quantum applications are going to play in tomorrow's society. **Quantum control** is one of the bricks of quantum engineering, and presents many peculiarities with respect to standard control theory, as a consequence of the specific properties of the systems described by the laws of quantum physics. Particularly important for technological applications is the capability of inducing and reproducing coherent state superpositions and entanglement in a fast, reliable, and efficient way [106].

3.2. Scientific foundations

At the core of the scientific activity of the team is the **geometric control** approach, that is, a distinctive viewpoint issued in particular from (elementary) differential geometry, to tackle questions of controllability, observability, optimal control... [68], [110]. The emphasis of such a geometric approach to control theory is put on intrinsic properties of the systems and it is particularly well adapted to study nonlinear and nonholonomic phenomena.

One of the features of the geometric control approach is its capability of exploiting **symmetries and intrinsic structures** of control systems. Symmetries and intrinsic structures can be used to characterize minimizing trajectories, prove regularity properties and describe invariants. An egregious example is given by mechanical systems, which inherently exhibit Lagrangian/Hamiltonian structures which are naturally expressed using the language of symplectic geometry [91]. The geometric theory of quantum control, in particular, exploits the rich geometric structure encoded in the Schrödinger equation to engineer adapted control schemes and to characterize their qualitative properties. The Lie–Galerkin technique that we proposed starting from 2009 [94] builds on this premises in order to provide powerful tests for the controllability of quantum systems defined on infinite-dimensional Hilbert spaces.

Although the focus of geometric control theory is on qualitative properties, its impact can also be disruptive when it is used in combination with quantitative analytical tools, in which case it can dramatically improve the computational efficiency. This is the case in particular in optimal control. Classical optimal control techniques (in particular, Pontryagin Maximum Principle, conjugate point theory, associated numerical methods) can be significantly improved by combining them with powerful modern techniques of geometric optimal control, of the theory of numerical continuation, or of dynamical system theory [152], [139]. Geometric optimal control allows the development of general techniques, applying to wide classes of nonlinear optimal control problems, that can be used to characterize the behavior of optimal trajectories and in particular to establish regularity properties for them and for the cost function. Hence, geometric optimal control can be used to obtain powerful optimal syntheses results and to provide deep geometric insights into many applied problems. Numerical optimal control methods with geometric insight are in particular important to handle subtle situations such as rigid optimal paths and, more generally, optimal syntheses exhibiting abnormal minimizers.

Optimal control is not the only area where the geometric approach has a great impact. Let us mention, for instance, motion planning, where different geometric approaches have been developed: those based on the **Lie algebra** associated with the control system [132], [121], those based on the differentiation of nonlinear flows such as the **return method** [99], [98], and those exploiting the **differential flatness** of the system [103].

Geometric control theory is not only a powerful framework to investigate control systems, but also a useful tool to model and study phenomena that are not *a priori* control-related. Two occurrences of this property play an important role in the activities of CAGE:

- geometric control theory as a tool to investigate properties of mathematical structures;

- geometric control theory as a modeling tool for neurophysical phenomena and for synthesizing biomimetic algorithms based on such models.

Examples of the first type, concern, for instance, hypoelliptic heat kernels [66] or shape optimization [74]. Examples of the second type are inactivation principles in human motricity [77] or neurogeometrical models for image representation of the primary visual cortex in mammals [88].

A particularly relevant class of control systems, both from the point of view of theory and applications, is characterized by the linearity of the controlled vector field with respect to the control parameters. When the controls are unconstrained in norm, this means that the admissible velocities form a distribution in the tangent bundle to the state manifold. If the distribution is equipped with a point-dependent quadratic form (encoding the cost of the control), the resulting geometrical structure is said to be **sub-Riemannian**. Sub-Riemannian geometry appears as the underlying geometry of nonlinear control systems: in a similar way as the linearization of a control system provides local informations which are readable using the Euclidean metric scale, sub-Riemannian geometry provides an adapted non-isotropic class of lenses which are often much more informative. As such, its study is fundamental for control design. The importance of sub-Riemannian geometry goes beyond control theory and it is an active field of research both in differential geometry [129], geometric measure theory [70] and hypoelliptic operator theory [80].

The geometric control approach has historically been related to the development of finite-dimensional control theory. However, its impact in the analysis of distributed parameter control systems and in particular systems of controlled partial differential equations has been growing in the last decades, complementing analytical and numerical approaches, providing dynamical, qualitative and intrinsic insight [97]. CAGE's ambition is to be at the core of this development in the years to come.

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 [28]), with improvements due to the "Chicago school", Bliss [20] during the first part of the 20th century, and by the notion of relaxed problem and generalized solution (Young [33]).

Trajectory optimization really started with the spectacular achievement done by Pontryagin's group [32] 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 [24], Leitmann [30], Lee and Markus [29], Ioffe and Tihomirov [27]).

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 [25]. The theoretical contributions in this direction did not cease growing, see the books by Barles [18] and Bardi and Capuzzo-Dolcetta [17].

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 [26], Bonnans [21]. 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 $I\!R^n$ (n is the number of state variables), and a methodology for finding an initial point.

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.

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.

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 [23]. 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 [22].

DISCO Project-Team

3. Research Program

3.1. Analysis of interconnected systems

The major questions considered are those of the characterization of the stability (also including the problems of sensitivity compared to the variations of the parameters) and the determination of stabilizing controllers of interconnected dynamic systems. In many situations, the dynamics of the interconnections can be naturally modelled by systems with delays (constant, distributed or time-varying delays) possibly of fractional order. In other cases, partial differential equations (PDE) models can be better represented or approximated by using systems with delays. Our expertise on this subject, on both time and frequency domain methods, allows us to challenge difficult problems (e.g. systems with an infinite number of unstable poles).

- Robust stability of linear systems

  Within an interconnection context, lots of phenomena are modelled directly or after an approximation by delay systems. These systems may have constant 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. [65]). 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.

3.2. Stabilization of interconnected systems

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

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

  A central issue studied in the team is the computation of such factorizations for a given infinite-dimensional linear system as well as establishing the links between stabilizability of a system for

a certain norm and the existence of coprime factorizations for this system. These questions are fundamental for robust stabilization problems [1], [2].

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

- Nonlinear systems

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

- Predictive control

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

  The team also investigates stochastic optimization methods such as genetic algorithm, particle swarm optimization or ant colony [8] as they can be used to optimize any criterion and constraint whatever their mathematical structure is. The developed methodologies can be used by non specialists.

3.3. Synthesis of reduced complexity controllers

- PID controllers

  Even though the synthesis of control laws of a given complexity is not a new problem, it is still open, even for finite-dimensional linear systems. Our purpose is to search for good families of “simple” (e.g. low order) controllers for infinite-dimensional dynamical systems. Within our approach, PID candidates are first considered in the team [2], [67].

- Predictive control

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

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

FACTAS Team

3. Research Program

3.1. Introduction

Within the extensive field of inverse problems, much of the research by Factas 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 [67]. 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 [75] 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 [31].

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 [69], [54]. 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, as well as convex relaxation of hyperbolic approximation problems, see Sections 3.2.2 and 6.2.2 .

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 [59] 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] [29], [79]. Such questions are particular instances of the so-called inverse potential problem, where a measure μ has to be recovered from the knowledge of the gradient of its potential (*i.e.*, the field) on part of a hypersurface (a curve in 2-D) encompassing the support of μ. For Laplace's operator, potentials are logarithmic in 2-D and Newtonian in higher dimensions. For elliptic operators with non constant coefficients, the potential depends on the form of fundamental solutions and is less manageable because it is no longer of convolution type. Nevertheless it is a useful concept bringing perspective on how problems could be raised and solved, using tools from harmonic analysis.

Inverse potential problems are severely indeterminate because infinitely many measures within an open set produce the same field outside this set; this phenomenon is called *balayage* [66]. In the two steps approach previously described, we implicitly removed this indeterminacy by requiring in step 1 that the measure be supported on the boundary (because we seek a function holomorphic throughout the right half-space), and by requiring in step 2 that the measure be discrete in the left half-plane (in fact: a sum of point masses $\sum_1^n a_j \delta_{z_j}$). The discreteness assumption also prevails in 3-D inverse source problems, see Section 4.3 . Conditions that ensure uniqueness of the solution to the inverse potential problem are part of the so-called regularizing assumptions which are needed in each case to derive efficient algorithms.

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

Along these lines, Factas advocates the use of steps 1 and 2 above, along with some singularity analysis, to approach issues of nondestructive control in 2-D and 3-D [2], [39], [42]. The team is currently engaged in the generalization to inverse source problems for the Laplace equation in 3-D, to be described further in Section 3.2.1 . There, holomorphic functions are replaced by harmonic gradients; applications are to inverse source problems in neurosciences (in particular in EEG/MEG) and inverse magnetization problems in geosciences, see Section 4.3 .

The approximation-theoretic tools developed by Apics and now by Factas 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.

Note that the Inria project-team Apics reached the end of its life cycle by the end of last year. The proposal for our new team Factas is since then being built and examined by the CEP (Comité des Équipes-Projets) of the Research Center, on its way to become a project-team.

3.2. Range of inverse problems

3.2.1. Elliptic partial differential equations (PDE)

Participants: Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Konstantinos Mavreas.

By standard properties of conjugate differentials, reconstructing Dirichlet-Neumann boundary conditions for a function harmonic in a plane domain, when these conditions are already known on a subset E of the boundary, is equivalent to recover a holomorphic function in the domain from its boundary values on E. This is the problem raised on the half-plane in step 1 of Section 3.1 . It makes good sense in holomorphic Hardy spaces where functions are entirely determined by their values on boundary subsets of positive linear measure, which is the framework for Problem (P) that we set up in Section 3.3.1 . Such issues naturally arise in nondestructive testing of 2-D (or 3-D cylindrical) materials from partial electrical measurements on

[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.

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 [52], [55].

Another application by the team deals with non-constant conductivity over a doubly connected domain, the set E being now the outer boundary. Measuring Dirichlet-Neumann data on E, one wants to recover level lines of the solution to a conductivity equation, which is a so-called free boundary inverse problem. For this, given a closed curve inside the domain, we first quantify how constant the solution on this curve. To this effect, we state and solve an analog of Problem (P), where the constraint bears on the real part of the function on the curve (it should be close to a constant there), in a Hardy space of a conjugate Beltrami equation, of which the considered conductivity equation is the compatibility condition (just like the Laplace equation is the compatibility condition of the Cauchy-Riemann system). Subsequently, a descent algorithm on the curve leads one to improve the initial guess. For example, when the domain is regarded as separating the edge of a tokamak's vessel from the plasma (rotational symmetry makes this a 2-D situation), this method can be used to estimate the shape of a plasma subject to magnetic confinement.

This was actually carried out in collaboration with CEA (French nuclear agency) and the University of Nice (JAD Lab.), to data from *Tore Supra* in [58]. 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 to the team.

The piece of work we just mentioned requires defining and studying Hardy spaces of conjugate Beltrami equations, which is an interesting topic. For Sobolev-smooth coefficients of exponent greater than 2, they were investigated in [5], [32]. The case of the critical exponent 2 is treated in [28], 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. More importantly perhaps, the exponent 2 is also the key to a corresponding theory on very general (still rectifiable) domains in the plane, as coefficients of pseudo-holomorphic functions obtained by conformal transformation onto a disk are merely of L^2-class in general, even if the initial problem deals with coefficients of L^r-class for some $r > 2$.

Generalized Hardy classes as above are used in [29] where we address the uniqueness issue in the classical Robin inverse problem on a Lipschitz domain of $\Omega \subset \mathbb{R}^n$, $n \geq 2$, with uniformly bounded Robin coefficient, L^2 Neumann data and conductivity of Sobolev class $W^{1,r}(\Omega)$, $r > n$. We show that uniqueness of the Robin coefficient on a subset of the boundary, given Cauchy data on the complementary part, does hold in dimension $n = 2$, thanks to a unique continuation result, but needs not hold in higher dimension. In higher dimension, this raises an open issue on harmonic gradients, namely whether the positivity of the Robin coefficient is compatible with identical vanishing of the boundary gradient on a subset of positive measure.

The 3-D version of step 1 in Section 3.1 is another subject investigated by Factas: to recover a harmonic function (up to an additive constant) in a ball or a half-space from partial knowledge of its gradient. This prototypical inverse problem (*i.e.* inverse to the Cauchy problem for the Laplace equation) often recurs in electromagnetism. At present, Factas 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], [35], see Section 6.1 . In this connection, we collaborate with two groups of partners: Athena Inria project-team and INS (Institut de Neurosciences des Systèmes, http://ins.univ-amu.fr/), hospital la Timone, Aix-Marseille Univ., on the one hand, Geosciences Lab. at MIT and Cerege CNRS Lab. on the other hand. The question is considerably more difficult than its 2-D counterpart, due mainly to the lack of multiplicative structure for harmonic gradients. Still, substantial progress has been made over the last years using methods of harmonic analysis and operator theory.

The team is further concerned with 3-D generalizations and applications to non-destructive control of step 2 in Section 3.1 . A typical problem is here to localize inhomogeneities or defaults such as cracks, sources or occlusions in a planar or 3-dimensional object, knowing thermal, electrical, or magnetic measurements on the boundary. These defaults can be expressed as a lack of harmonicity of the solution to the associated Dirichlet-Neumann problem, thereby posing an inverse potential problem in order to recover them. In 2-D, finding an optimal discretization of the potential in Sobolev norm amounts to solve a best rational approximation problem, and the question arises as to how the location of the singularities of the approximant (*i.e.* its poles) reflects the location of the singularities of the potential (*i.e.* the defaults we seek). This is a fairly deep issue in approximation theory, to which Apics contributed convergence results for certain classes of fields expressed as Cauchy integrals over extremal contours for the logarithmic potential [7], [36], [49]. Initial schemes to locate cracks or sources *via* rational approximation on planar domains were obtained this way [39], [42], [52]. 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 [8], [40]. More precisely, each section cuts out a planar domain, the boundary of which carries data which can be proved to match an algebraic function. The singularities of this algebraic function are not located at the 3-D sources, but are related to them: the section contains a source if and only if some function of the singularities in that section meets a relative extremum. Using bisection it is thus possible to determine an extremal place along all sections parallel to a given plane direction, up to some threshold which has to be chosen small enough that one does not miss a source. This way, we reduce the original source problem in 3-D to a sequence of inverse poles and branchpoints problems in 2-D. This bottom line generates a steady research activity within Factas, and again applications are sought to medical imaging and geosciences, see Sections 4.3 , 4.2 and 6.1 .

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

3.2.2. Systems, transfer and scattering

Participants: Laurent Baratchart, Sylvain Chevillard, Adam Cooman, Martine Olivi, Fabien Seyfert.

Through contacts with CNES (French space agency), members of the team became involved in identification and tuning of microwave electromagnetic filters used in space telecommunications, see Section 4.4 . The initial problem was to recover, from band-limited frequency measurements, physical parameters of the device under examination. The latter consists of interconnected dual-mode resonant cavities with negligible loss, hence its scattering matrix is modeled by a 2×2 unitary-valued matrix function on the frequency line, say the imaginary axis to fix ideas. In the bandwidth around the resonant frequency, a modal approximation of the Helmholtz equation in the cavities shows that this matrix is approximately rational, of Mc-Millan degree twice the number of cavities.

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

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

1. infer from the pointwise boundary data in the bandwidth a stable transfer function (*i.e.* one which is holomorphic in the right half-plane), that may be infinite dimensional (numerically: of high degree). This is done by solving a problem analogous to (P) in Section 3.3.1 , while taking into account prior knowledge on the decay of the response outside the bandwidth, see [11] 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 [24], [11].

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 [53], as solving a zero-dimensional multivariate polynomial system. To tackle this problem in practice, we use Gröbner basis techniques and continuation methods which team up in the Dedale-HF software (see Section 3.4.1).

Let us mention that extensions of classical coupling matrix theory to frequency-dependent (reactive) couplings have been carried-out in recent years [1] for wide-band design applications.

Factas also investigates issues pertaining to design rather than identification. Given the topology of the filter, a basic problem in this connection is to find the optimal response subject to specifications that bear on rejection, transmission and group delay of the scattering parameters. Generalizing the classical approach based on Chebyshev polynomials for single band filters, we recast the problem of multi-band response synthesis as a generalization of the classical Zolotarev min-max problem for rational functions [23] [10]. Thanks to quasi-convexity, the latter can be solved efficiently using iterative methods relying on linear programming. These were implemented in the software easy-FF (see easy-FF). Currently, the team is engaged in the synthesis of more complex microwave devices like multiplexers and routers, which connect several filters through wave guides. Schur analysis plays an important role here, because scattering matrices of passive systems are of Schur type (*i.e.* contractive in the stability region). The theory originates with the work of I. Schur [74], 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 [25]. Dwelling on this, Factas contributed differential parametrizations (atlases of charts) of lossless matrix functions [24], [68], [63] which are fundamental to our rational approximation software RARL2 (see Section 3.4.4). Schur analysis is also instrumental to approach de-embedding issues, and provides one with considerable insight into the so-called matching problem. The latter consists in maximizing the power a multiport can pass to a given load, and for reasons of efficiency it is all-pervasive in microwave and electric network design, *e.g.* of antennas, multiplexers, wifi cards and more. It can be viewed as a rational approximation problem in the hyperbolic metric, and the team presently deals with this hot topic using contractive interpolation with constraints on boundary peak points, within the framework of the (defense funded) ANR Cocoram, see Sections 6.2 and 8.2.2 .

In recent years, our attention was driven by CNES and UPV (Bilbao) to questions about stability of high-frequency amplifiers. Contrary to previously discussed devices, these are *active* components. The response of an amplifier can be linearized around a set of primary current and voltages, and then admittances of the corresponding electrical network can be computed at various frequencies, using the so-called harmonic balance method. The initial goal is to check for stability of the linearized model, so as to ascertain existence of a well-defined working state. The network is composed of lumped electrical elements namely inductors, capacitors, negative *and* positive reactors, transmission lines, and controlled current sources. Our research so far has focused on describing the algebraic structure of admittance functions, so as to set up a function-theoretic framework where the two-steps approach outlined in Section 3.1 can be put to work. The main discovery is that the unstable part of each partial transfer function is rational and can be computed by analytic projection, see Section 6.3 . We now start investigating the linearized harmonic transfer-function around a periodic cycle, to check for stability under non necessarily small inputs. This generalization generates both doctoral and postdoctoral work by new students in the team.

3.3. Approximation

Participants: Laurent Baratchart, Sylvain Chevillard, Juliette Leblond, Martine Olivi, Fabien Seyfert.

3.3.1. Best analytic approximation

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

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

> (P) Let $1 \leq p \leq \infty$, 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 $\|g - \psi\|_{L^p(T \setminus K)} \leq M$ and $g - f$ is of minimal norm in $L^p(K)$ under this constraint.

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

To fix terminology, we refer to (P) as a *bounded extremal problem*. As shown in [38], [41], [46], 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 [61]:

> (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 tailored to meet specific needs. For instance when dealing with lossless transfer functions (see Section 4.4), one may want to express the constraint on $T \setminus K$ in a pointwise manner: $|g - \psi| \leq M$ a.e. on $T \setminus K$, see [13]. In this form, the problem comes close to (but still is different from) H^∞ frequency optimization used in control [64], [73]. One can also impose bounds on the real or imaginary part of $g - \psi$ on $T \setminus K$, which is useful when considering Dirichlet-Neumann problems.

The analog of Problem (P) on an annulus, K being now the outer boundary, can be seen as a means to regularize a classical inverse problem occurring in nondestructive control, namely to recover a harmonic function on the inner boundary from Dirichlet-Neumann data on the outer boundary (see Sections 3.2.1 , 4.3 , 6.1.3). It may serve as a tool to approach Bernoulli type problems, where we are given data on the outer boundary and we *seek the inner boundary*, knowing it is a level curve of the solution. In this case, the Lagrange parameter indicates how to deform the inner contour in order to improve data fitting. Similar topics are discussed in Section 3.2.1 for more general equations than the Laplacian, namely isotropic conductivity equations of the form $\mathrm{div}(\sigma \nabla u) = 0$ where σ is no longer constant. Then, the Hardy spaces in Problem (P) are those of a so-called conjugate Beltrami equation: $\overline{\partial} f = \nu \overline{\partial f}$ [65], which are studied for $1 < p < \infty$ in [5], [28], [32] and [56]. Expansions of solutions needed to constructively handle such issues in the specific case of linear fractional conductivities (occurring for instance in plasma shaping) have been expounded in [58].

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

When Ω is a ball or a half-space, a substitute for holomorphic Hardy spaces is provided by the Stein-Weiss Hardy spaces of harmonic gradients [77]. Conformal maps are no longer available when $n > 2$, so that Ω can no longer be normalized. More general geometries than spheres and half-spaces have not been much studied so far.

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

> (P_1) Let $1 \leq p \leq \infty$ 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, when the tangent component of V is a gradient (when O is Lipschitz the general case follows easily from this). The solution extends the work in [38] to the 3-D case, using a generalization of Toeplitz operators. The case of the shell was motivated by applications to the processing of EEG data. An important ingredient is a refinement of the Hodge decomposition, that we call the *Hardy-Hodge* decomposition, allowing us to express a $\mathbb{R}^n$-valued vector field in $L^p(S)$, $1 < p < \infty$, as the sum of a vector field in $H^p(B)$, a vector field in $H^p(\mathbb{R}^n \setminus \overline{B})$, and a tangential divergence free vector field on S; the space of such divergence-free fields is denoted by $D(S)$. If $p = 1$ or $p = \infty$, L^p must be replaced by the real Hardy space or the space of functions with bounded mean oscillation. More generally this decomposition, which is valid on any sufficiently smooth surface (see Section 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) [35].

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

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

Problem (P_2) is simple when $p = 2$ by virtue of the Hardy-Hodge decomposition together with orthogonality of $H^2(B)$ and $H^2(\mathbb{R}^n \setminus \overline{B})$, which is the reason why we were able to solve (P_1) in this case. Other values of p cannot be treated as easily and are still under investigation, especially the case $p = \infty$ which is of particular interest and presents itself as a 3-D analog to the Nehari problem [71].

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

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

Note that (P_2) and (P_3) are identical in 2-D, since no non-constant tangential divergence-free vector field exists on T. It is no longer so in higher dimension, where both (P_2) and (P_3) arise in connection with inverse potential problems in divergence form, like source recovery in electro/magneto encephalography and paleomagnetism, see Sections 3.2.1 and 4.3 .

3.3.2. Best meromorphic and rational approximation

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

3.3.2.1. Scalar meromorphic and rational approximation

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

A natural generalization of problem (P_0) is:

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

Only for $p = \infty$ and f continuous is it known how to solve (P_N) in semi-closed form. The unique solution is given by AAK theory (named after Adamjan, Arov and Krein), which connects the spectral decomposition of Hankel operators with best approximation [71].

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 [30]. Although it has proved to be effective in all applications carried out so far (see Sections 4.3 , 4.4), it is still unknown whether the absolute minimum can always be obtained by choosing initial conditions corresponding to *critical points* of lower degree (as is done by the RARL2 software, Section 3.4.4).

In order to establish global convergence results, Apics has undertaken a deeper study of the number and nature of critical points (local minima, saddle points, ...), in which tools from differential topology and operator theory team up with classical interpolation theory [43], [45]. 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) [47] and more generally Cauchy integrals over hyperbolic geodesic arcs [50]. 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 [26] in higher dimension is a worthy and timely endeavor today. Meanwhile, an analog to AAK theory was carried out for $2 \leq p < \infty$ in [46]. Although not as effective computationally, it was recently used to derive lower bounds [4]. 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 [51], [48], and is used in an essential manner to assess the behavior of poles of best approximants to functions with branched singularities, which is of particular interest for inverse source problems (*cf.* Sections 3.4.2 and 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 field of research. It is connected with certain generalizations of Toeplitz or Hankel operators, and with constructive approaches to so-called weak factorizations for real Hardy functions [57].

Besides, certain constrained rational approximation problems, of special interest in identification and design of passive systems, arise when putting additional requirements on the approximant, for instance that it should be smaller than 1 in modulus (*i.e.* a Schur function). In particular, Schur interpolation lately received renewed attention from the team, in connection with matching problems. There, interpolation data are subject to a well-known compatibility condition (positive definiteness of the so-called Pick matrix), and the main difficulty is to put interpolation points on the boundary of D while controlling both the degree and the extremal points (peak points for the modulus) of the interpolant. Results obtained by Apics in this direction generalize a variant of contractive interpolation with degree constraint as studied in [62]. 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 [34], [37].

3.3.2.2. Matrix-valued rational approximation

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

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

The scalar approximation algorithm derived in [30] and mentioned in Section 3.3.2.1 generalizes to the matrix-valued situation [60]. 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 ([24], [63], [68]). Some of these parametrizations are also interesting to compute realizations and achieve filter synthesis ([63], [68]). The rational approximation software "RARL2" developed by the team is described in Section 3.4.4 .

Difficulties relative to multiple local minima of course arise in the matrix-valued case as well, and deriving criteria that guarantee uniqueness is even more difficult than in the scalar case. The case of rational functions of degree n or small perturbations thereof (the consistency problem) was solved in [44]. Matrix-valued Markov functions are the only known example beyond this one [27].

Let us stress that RARL2 seems the only algorithm handling rational approximation in the matrix case that demonstrably converges to a local minimum while meeting stability constraints on the approximant. It is still a working pin of many developments by Factas on frequency optimization and design.

3.3.3. Behavior of poles of meromorphic approximants

Participant: Laurent Baratchart.

We refer here to the behavior of poles of best meromorphic approximants, in the L^p-sense on a closed curve, to functions f defined as Cauchy integrals of complex measures whose support lies inside the curve. Normalizing the contour to be the unit circle T, we are back to Problem (P_N) in Section 3.3.2.1 ; invariance of the latter under conformal mapping was established in [42]. Research so far has focused on functions whose singular set inside the contour is polar, meaning that the function can be continued analytically (possibly in a multiple-valued manner) except over a set of logarithmic capacity zero.

Generally speaking in approximation theory, assessing the behavior of poles of rational approximants is essential to obtain error rates as the degree goes large, and to tackle constructive issues like uniqueness. However, as explained in Section 3.2.1 , the original twist by Apics, now Factas, is to consider this issue also as a means to extract information on singularities of the solution to a Dirichlet-Neumann problem. The general theme is thus: *how do the singularities of the approximant reflect those of the approximated function?* This approach to inverse problem for the 2-D Laplacian turns out to be attractive when singularities are zero- or one-dimensional (see Section 4.3). It can be used as a computationally cheap initial condition for more precise but much heavier numerical optimizations which often do not even converge unless properly initialized. As regards crack detection or source recovery, this approach boils down to analyzing the behavior of best meromorphic approximants of given pole cardinality to a function with branch points, which is the prototype of a polar singular set. For piecewise analytic cracks, or in the case of sources, we were able to prove ([7], [42], [36]), 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 [39]. 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 3.4.2 .

3.4. Software tools of the team

In addition to the above-mentioned research activities, Factas develops and maintains a number of long-term software tools that either implement and illustrate effectiveness of the algorithms theoretically developed by the team or serve as tools to help further research by team members. We present briefly the most important of them.

3.4.1. DEDALE-HF

SCIENTIFIC DESCRIPTION

Dedale-HF consists in two parts: a database of coupling topologies as well as a dedicated predictor-corrector code. Roughly speaking each reference file of the database contains, for a given coupling topology, the complete solution to the coupling matrix synthesis problem (C.M. problem for short) associated to particular filtering characteristics. The latter is then used as a starting point for a predictor-corrector integration method that computes the solution to the C.M. corresponding to the user-specified filter characteristics. The reference files are computed off-line using Gröbner basis techniques or numerical techniques based on the exploration of a monodromy group. The use of such continuation techniques, combined with an efficient implementation of the integrator, drastically reduces the computational time.

Dedale-HF has been licensed to, and is currently used by TAS-Espana

FUNCTIONAL DESCRIPTION

Dedale-HF is a software dedicated to solve exhaustively the coupling matrix synthesis problem in reasonable time for the filtering community. Given a coupling topology, the coupling matrix synthesis problem consists in finding all possible electromagnetic coupling values between resonators that yield a realization of given filter characteristics. Solving the latter is crucial during the design step of a filter in order to derive its physical dimensions, as well as during the tuning process where coupling values need to be extracted from frequency measurements.

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- URL: http://www-sop.inria.fr/apics/Dedale/

3.4.2. FindSources3D

KEYWORDS: Health - Neuroimaging - Visualization - Compilers - Medical - Image - Processing

FindSources3D is a software program dedicated to the resolution of inverse source problems in electroencephalography (EEG). From pointwise measurements of the electrical potential taken by electrodes on the scalp, FindSources3D estimates pointwise dipolar current sources within the brain in a spherical model.

After a first data transmission “cortical mapping” step, it makes use of best rational approximation on 2-D planar cross-sections and of the software RARL2 in order to locate singularities. From those planar singularities, the 3-D sources are estimated in a last step, see [8].

The present version of FindSources3D (called FindSources3D-bolis) provides a modular, ergonomic, accessible and interactive platform, with a convenient graphical interface and a tool that can be distributed and used, for EEG medical imaging. Modularity is now granted (using the tools dtk, Qt, with compiled Matlab libraries). It offers a detailed and nice visualization of data and tuning parameters, processing steps, and of the computed results (using VTK).

A new version is being developed that will incorporate a first Singular Value Decomposition (SVD) step in order to be able to handle time dependent data and to find the corresponding principal static components.

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- URL: http://www-sop.inria.fr/apics/FindSources3D/en/index.html

3.4.3. PRESTO-HF

SCIENTIFIC DESCRIPTION

For the matrix-valued rational approximation step, Presto-HF relies on RARL2. Constrained realizations are computed using the Dedale-HF software. As a toolbox, Presto-HF has a modular structure, which allows one for example to include some building blocks in an already existing software.

The delay compensation algorithm is based on the following assumption: far off the pass-band, one can reasonably expect a good approximation of the rational components of S11 and S22 by the first few terms of their Taylor expansion at infinity, a small degree polynomial in 1/s. Using this idea, a sequence of quadratic convex optimization problems are solved, in order to obtain appropriate compensations. In order to check the previous assumption, one has to measure the filter on a larger band, typically three times the pass band.

This toolbox has been licensed to, and is currently used by Thales Alenia Space in Toulouse and Madrid, Thales airborne systems and Flextronics (two licenses). XLIM (University of Limoges) is a heavy user of Presto-HF among the academic filtering community and some free license agreements have been granted to the microwave department of the University of Erlangen (Germany) and the Royal Military College (Kingston, Canada).

FUNCTIONAL DESCRIPTION

Presto-HF is a toolbox dedicated to low-pass parameter identification for microwave filters. In order to allow the industrial transfer of our methods, a Matlab-based toolbox has been developed, dedicated to the problem of identification of low-pass microwave filter parameters. It allows one to run the following algorithmic steps, either individually or in a single stroke:

• Determination of delay components caused by the access devices (automatic reference plane adjustment),

• Automatic determination of an analytic completion, bounded in modulus for each channel,

• Rational approximation of fixed McMillan degree,

• Determination of a constrained realization.

- Participants: Fabien Seyfert, Jean-Paul Marmorat and Martine Olivi
- Contact: Fabien Seyfert
- URL: https://project.inria.fr/presto-hf/

3.4.4. RARL2

Réalisation interne et Approximation Rationnelle L2

SCIENTIFIC DESCRIPTION

The method is a steepest-descent algorithm. A parametrization of MIMO systems is used, which ensures that the stability constraint on the approximant is met. The implementation, in Matlab, is based on state-space representations.

RARL2 performs the rational approximation step in the software tools PRESTO-HF and FindSources3D. It is distributed under a particular license, allowing unlimited usage for academic research purposes. It was released to the universities of Delft and Maastricht (the Netherlands), Cork (Ireland), Brussels (Belgium), Macao (China) and BITS-Pilani Hyderabad Campus (India).

FUNCTIONAL DESCRIPTION

RARL2 is a software for rational approximation. It computes a stable rational L2-approximation of specified order to a given L2-stable (L2 on the unit circle, analytic in the complement of the unit disk) matrix-valued function. This can be the transfer function of a multivariable discrete-time stable system. RARL2 takes as input either:

• its internal realization,

• its first N Fourier coefficients,

• discretized (uniformly distributed) values on the circle. In this case, a least-square criterion is used instead of the L2 norm.

It thus performs model reduction in the first or the second case, and leans on frequency data identification in the third. For band-limited frequency data, it could be necessary to infer the behavior of the system outside the bandwidth before performing rational approximation.

An appropriate Möbius transformation allows to use the software for continuous-time systems as well.

- Participants: Jean-Paul Marmorat and Martine Olivi
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- URL: http://www-sop.inria.fr/apics/RARL2/rarl2.html

3.4.5. Sollya

KEYWORDS: Numerical algorithm - Supremum norm - Curve plotting - Remez algorithm - Code generator - Proof synthesis
FUNCTIONAL DESCRIPTION

Sollya is an interactive tool where the developers of mathematical floating-point libraries (libm) can experiment before actually developing code. The environment is safe with respect to floating-point errors, i.e. the user precisely knows when rounding errors or approximation errors happen, and rigorous bounds are always provided for these errors.

Among other features, it offers a fast Remez algorithm for computing polynomial approximations of real functions and also an algorithm for finding good polynomial approximants with floating-point coefficients to any real function. As well, it provides algorithms for the certification of numerical codes, such as Taylor Models, interval arithmetic or certified supremum norms.

It is available as a free software under the CeCILL-C license.

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- Contact: Sylvain Chevillard
- URL: http://sollya.gforge.inria.fr/

I4S Project-Team

3. Research Program

3.1. Vibration analysis

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

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

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

3.1.1. Identification

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

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

$$\left\{\begin{array}{rcl} X_{k+1} & = & F\ X_k + V_{k+1} \\ Y_k & = & H\ X_k + W_k \end{array}\right. , \tag{9}$$

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

$$\det\ (F-\lambda\ I)=0,\quad (F-\lambda\ I)\ \phi_\lambda=0,\quad \varphi_\lambda\stackrel{\Delta}{=}H\ \phi_\lambda \tag{10}$$

The (canonical) parameter vector in that case is :

$$\theta\stackrel{\Delta}{=}\left(\begin{array}{c}\Lambda\\ \mathrm{vec}\Phi\end{array}\right) \tag{11}$$

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 [57].

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

$$\mathcal{H}_{p+1,q} \triangleq \begin{pmatrix} R_1 & R_2 & \vdots & R_q \\ R_2 & R_3 & \vdots & R_{q+1} \\ \vdots & \vdots & \vdots & \vdots \\ R_{p+1} & R_{p+2} & \vdots & R_{p+q} \end{pmatrix} \triangleq \text{Hank}\left(R_i\right) \tag{12}$$

be the output covariance and Hankel matrices, respectively; and: $G \triangleq \mathbf{E}\left(X_k Y_{k-1}^T\right)$. Direct computations of the R_i's from the equations (4) lead to the well known key factorizations :

$$\begin{array}{rcl} R_i & = & HF^{i-1}G \\ \mathcal{H}_{p+1,q} & = & \mathcal{O}_{p+1}(H,F)\ \mathcal{C}_q(F,G) \end{array} \tag{13}$$

where:

$$\mathcal{O}_{p+1}(H,F) \triangleq \begin{pmatrix} H \\ HF \\ \vdots \\ HF^p \end{pmatrix} \quad \text{and} \quad \mathcal{C}_q(F,G) \triangleq (G\ FG\ \cdots\ F^{q-1}G) \tag{14}$$

are the observability and controllability matrices, respectively. The observation matrix H is then found in the first block-row of the observability matrix $\mathcal{O}$. The state-transition matrix F is obtained from the shift invariance property of $\mathcal{O}$. The eigenstructure (λ, ϕ_λ) then results from (5).

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

3.1.2. Detection

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

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

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

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

Choosing the eigenvectors of matrix F as a basis for the state space of model (4) yields the following representation of the observability matrix:

$$\mathcal{O}_{p+1}(\theta) = \begin{pmatrix} \Phi \\ \Phi\Delta \\ \vdots \\ \Phi\Delta^p \end{pmatrix} \tag{15}$$

where $\Delta \triangleq \mathrm{diag}(\Lambda)$, and Λ and Φ are as in (6). Whether a nominal parameter θ_0 fits a given output covariance sequence $(R_j)_j$ is characterized by:

$$\mathcal{O}_{p+1}(\theta_0) \text{ and } \mathcal{H}_{p+1,q} \text{ have the same left kernel space.} \tag{16}$$

This property can be checked as follows. From the nominal θ_0, compute $\mathcal{O}_{p+1}(\theta_0)$ using (10), and perform e.g. a singular value decomposition (SVD) of $\mathcal{O}_{p+1}(\theta_0)$ for extracting a matrix U such that:

$$U^T\, U = I_s \text{ and } U^T\, \mathcal{O}_{p+1}(\theta_0) = 0 \tag{17}$$

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:

$$U(\theta_0)^T\, \mathcal{H}_{p+1,q} = 0 \tag{18}$$

3.1.2.1. Residual associated with subspace identification.

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

$$\widehat{\mathcal{H}}_{p+1,q} \triangleq \mathrm{Hank}\left(\widehat{R}_i\right), \quad \widehat{R}_i \triangleq 1/(N-i) \sum_{k=i+1}^{N} Y_k\, Y_{k-i}^T \tag{19}$$

and to define the residual vector:

$$\zeta_N(\theta_0) \triangleq \sqrt{N}\ \mathrm{vec}\left(U(\theta_0)^T\, \widehat{\mathcal{H}}_{p+1,q}\right) \tag{20}$$

Let θ be the actual parameter value for the system which generated the new data sample, and $\mathbf{E}_\theta$ be the expectation when the actual system parameter is θ. From (13), we know that $\zeta_N(\theta_0)$ has zero mean when no change occurs in θ, and nonzero mean if a change occurs. Thus $\zeta_N(\theta_0)$ plays the role of a residual.

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

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

The central limit theorem shows [51] that the residual is asymptotically Gaussian :

$$\zeta_N \xrightarrow[N \to \infty]{} \begin{cases} \mathcal{N}(0, \Sigma) & \text{under } \mathbf{P}_{\theta_0} \ , \\ \\ \mathcal{N}(\mathcal{J}\,\eta, \Sigma) & \text{under } \mathbf{P}_{\theta_0 + \eta/\sqrt{N}} \ , \end{cases} \tag{21}$$

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 :

$$\chi^2 = \overline{\zeta}^{\,T}\, \mathbf{F}^{-1}\, \overline{\zeta} \gtrless \lambda \ . \tag{22}$$

where

$$\overline{\zeta} \triangleq \mathcal{J}^T\, \Sigma^{-1}\, \zeta_N \quad \text{and} \quad \mathbf{F} \triangleq \mathcal{J}^T\, \Sigma^{-1}\, \mathcal{J} \tag{23}$$

3.1.3. Diagnostics

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

The question: *which (subsets of) components of θ have changed ?*, can be addressed using either nuisance parameters elimination methods or a multiple hypotheses testing approach [50].

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

The isolation methods sketched above are possible solutions to the former. Our approach to the latter diagnosis problem is basically a detection approach again, and not a (generally ill-posed) inverse problem estimation approach.

The basic idea is to note that the physical sensitivity matrix writes $\mathcal{J}\,\mathcal{J}_{\Phi\theta}$, where $\mathcal{J}_{\Phi\theta}$ is the Jacobian matrix at Φ_0 of the application $\Phi \mapsto \theta(\Phi)$, and to use the sensitivity test for the components of the parameter vector Φ. Typically this results in the following type of directional test :

$$\chi^2_\Phi = \zeta^T\, \Sigma^{-1}\, \mathcal{J}\, \mathcal{J}_{\Phi\theta}\, \left(\mathcal{J}_{\Phi\theta}^T\, \mathcal{J}^T\, \Sigma^{-1}\, \mathcal{J}\, \mathcal{J}_{\Phi\theta}\right)^{-1} \mathcal{J}_{\Phi\theta}^T\, \mathcal{J}^T\, \Sigma^{-1}\, \zeta \gtrless \lambda \ . \tag{24}$$

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

3.2. Thermal methods

3.2.1. Infrared thermography and heat transfer

This section introduces the infrared radiation and its link with the temperature, in the next part different measurement methods based on that principle are presented.

3.2.1.1. Infrared radiation

Infrared is an electromagnetic radiation having a wavelength between $0.2\mu m$ and $1\ mm$, this range begin in uv spectrum and it ends on the microwaves domain, see Figure 1 .

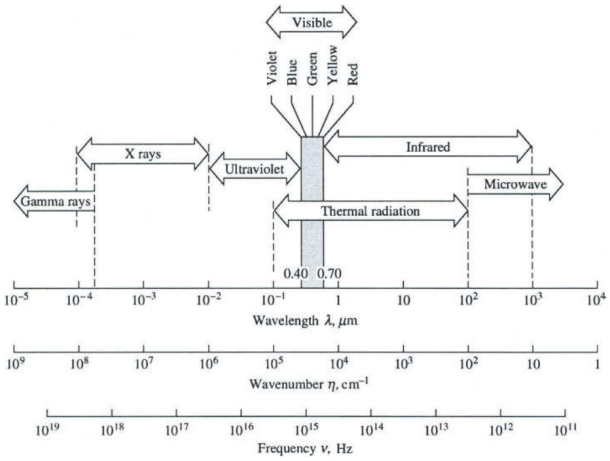

Figure 1. Electromagnetic spectrum - Credit MODEST, M.F. (1993). Radiative Heat Transfer. Academic Press.

For scientific purposes, infrared can be divided in three ranges of wavelength in which the application varies, see Table 1 .

Table 1. Wavelength bands in the infrared according to ISO 20473:2007

Band name	**wavelength**	**Uses ⟍ definition**
Near infrared (PIR, IR-A, NIR)	$0.7 - 3\mu$m	Reflected solar heat flux
Mid infrared (MIR, IR-B)	$3 - 50\mu$m	Thermal infrared
Far infrared (LIR, IR-C, FIR)	$50 - 1000\mu$m	Astronomy

Our work is concentrated in the mid infrared spectral band. Keep in mind that Table 1 represents the ISO 20473 division scheme, in the literature boundaries between bands can move slightly.
The Plank's law, proposed by Max Planck in 1901, allows to compute the black body emission spectrum for various temperatures (and only temperatures), see Figure 2 left. The black body is a theoretical construction, it represents perfect energy emitter at a given temperature, cf. Equation (20).

$$M^o_{\lambda,T} = \frac{C_1 \lambda^{-5}}{\exp^{\frac{C_2}{\lambda T}} - 1} \tag{25}$$

With λ the wavelength in m and T as the temperature in Kelvin. The C_1 and C_2 constants, respectively in W.m^2 and m.K are defined as follow:

$$\begin{aligned} C_1 &= 2hc^2\pi \\ C_2 &= h\frac{c}{k} \end{aligned} \tag{26}$$

with

- c, the electromagnetic wave speed (in vacuum c is the light speed in m.s^{-1}).
- $k = 1.381e^{-23}$ J.K^{-1} The Boltzmann (Entropy definition from Ludwig Boltzmann 1873). It can be seen as a proportionality factor between the temperature and the energy of a system.
- $h \approx 6,62606957e^{-34}$ J.s The Plank constant. It is the link between the photons energy and their frequency.

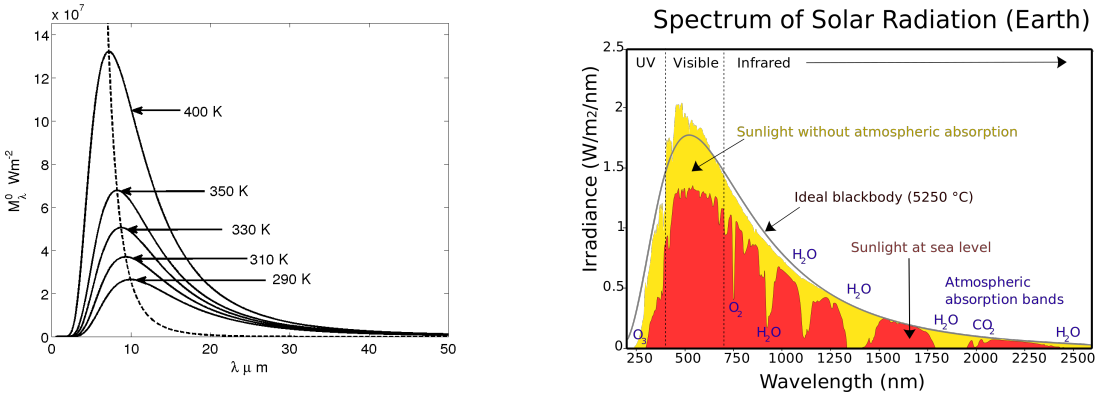

Figure 2. Left: Plank's law at various temperatures - Right: Energy spectrum of the atmosphere

By generalizing the Plank's law with the Stefan Boltzmann law (proposed first in 1879 and then in 1884 by Joseph Stefan and Ludwig Boltzmann), it is possible to address mathematically the energy spectrum of real body at each wavelength depending on the temperature, the optical condition and the real body properties, which is the base of the infrared thermography.

For example, Figure 2 right presents the energy spectrum of the atmosphere at various levels, it can be seen that the various properties of the atmosphere affect the spectrum at various wavelengths. Other important point is that the infrared solar heat flux can be approximated by a black body at 5523,15 K.

3.2.1.2. Infrared Thermography

The infrared thermography is a way to measure the thermal radiation received from a medium. With that information about the electromagnetic flux, it is possible to estimate the surface temperature of the body, see section 3.2.1.1 . Various types of detector can assure the measure of the electromagnetic radiation.

Those different detectors can take various forms and/or manufacturing process. For our research purposes, we use uncooled infrared camera using a matrix of microbolometers detectors. A microbolometer, as a lot of transducers, converts a radiation in electric current used to represent the physical quantity (here the heat flux).

This field of activity includes the use and the improvement of vision system, like in [3].

3.2.2. Heat transfer theory

Once the acquisition process is done, it is useful to model the heat conduction inside the cartesian domain Ω. Note that in opaque solid medium the heat conduction is the only mode of heat transfer. Proposed by Jean Baptiste Biot in 1804 and experimentally demonstrated by Joseph Fourier in 1821, the Fourier Law describes the heat flux inside a solid, cf Equation (22).

$$\varphi = k\nabla T \quad X \in \Omega \tag{27}$$

Where k is the thermal conductivity in W.m^{-1}.K ^{o}, ∇ is the gradient operator and φ is the heat flux density in Wm^{-2}. This law illustrates the first principle of thermodynamic (law of conservation of energy) and implies the second principle (irreversibility of the phenomenon). From this law it can be seen that the heat flux always goes from hot area to cold area.
An energy balance with respect to the first principle yields to the expression of the heat conduction in all point of the domain Ω, cf Equation (23). This equation has been proposed by Joseph Fourier in 1811.

$$\rho C \frac{\partial T(X,t)}{\partial t} = \nabla \cdot (k \nabla T) + P \quad X \in \Omega \tag{28}$$

With $\nabla.()$ the divergence operator, C the specific heat capacity in J.kg^{-1}.^{o}K^{-1}, ρ the volumetric mass density in kg. m^{-3}, X the space variable $X = \{x, y, z\}$ and P a possible internal heat production in W.m^{-3}.
To solve the system (23), it is necessary to express the boundaries conditions of the system. With the developments presented in section 3.2.1.1 and the Fourier's law, it is possible, for example, to express the thermal radiation and the convection phenomenon which can occur at $\partial\Omega$ the system boundaries, cf Equation (24).

$$\varphi = k \nabla T \cdot n = \underbrace{h \left(T_{fluid} - T_{Boundarie}\right)}_{\text{Convection}} + \underbrace{\epsilon \sigma_s \left(T^4_{environement} - T^4_{Boundary}\right)}_{\text{Radiation}} + \varphi_0 \quad X \in \partial\Omega \tag{29}$$

Equation (24) is the so called Robin condition on the boundary $\partial\Omega$, where n is the normal, h the convective heat transfer coefficient in W.m^{-2}.K^{-1} and φ_0 an external energy contribution W.m^{-2}, in cases where the external energy contribution is artificial and controlled we call it active thermography (spotlight etc...), otherwise it is called passive thermography (direct solar heat flux).
The systems presented in the different sections above (3.2.1 to 3.2.2) are useful to build physical models in order to represents the measured quantity. To estimate key parameters, as the conductivity, model inversion is used, the next section will introduce that principle.

3.2.3. Inverse model for parameters estimation

Lets take any model A which can for example represent the conductive heat transfer in a medium, the model is solved for a parameter vector P and it yields another vector b, cf Equation (25). For example if A represents the heat transfer, b can be the temperature evolution.

$$AP = b \tag{30}$$

With A a matrix of size $n \times m$, P a vector of size m and b of size n, preferentially $n >> P$. This model is called direct model, the inverse model consist to find a vector P which satisfy the results b of the direct model. For that we need to inverse the matrix A, cf Equation (26).

$$P = A^{-1} b \tag{31}$$

Here we want to find the solution AP which is closest to the acquired measures M, Equation (27).

$$AP \approx \mathcal{M} \tag{32}$$

To do that it is important to respect the well posed condition established by Jacques Hadamard in 1902

- A solution exists.
- The solution is unique.
- The solution's behavior changes continuously with the initial conditions.

Unfortunately those condition are rarely respected in our field of study. That is why we dont solve directly the system (27) but we minimise the quadratic coast function (28) which represents the Legendre-Gauss least square algorithm for linear problems.

$$min_P \left(\|AP - \mathcal{M}\|^2 \right) = min_P \left(\mathcal{F} \right) \tag{33}$$

Where $\mathcal{F}$ can be a product of matrix.

$$\mathcal{F} = \left[AP - \mathcal{M} \right]^T \left[AP - \mathcal{M} \right]$$

In some cases the problem is still ill-posed and need to be regularized for example using the Tikhonov regularization. An elegant way to minimize the cost function $\mathcal{F}$ is compute the gradient, Equation (29) and find where it is equal to zero.

$$\nabla \mathcal{F}(P) = 2 \left[-\frac{\partial A P^T}{\partial P} \right] \left[AP - \mathcal{M} \right] = 2 J(P)^T \left[AP - \mathcal{M} \right] \tag{34}$$

Where J is the sensitivity matrix of the model A with respect to the parameter vector P.
Until now the inverse method proposed is valid only when the model A is linearly dependent of its parameter P, for the heat equation it is the case when the external heat flux has to be estimated, φ_0 in Equation (24). For all the other parameters, like the conductivity k the model is non-linearly dependant of its parameter P. For such case the use of iterative algorithm is needed, for example the Levenberg-Marquardt algorithm, cf Equation (30).

$$P^{k+1} = P^k + \left[\left(J^k \right)^T J^k + \mu^k \Omega^k \right]^{-1} \left(J^k \right)^T \left[\mathcal{M} - A(P^k) \right] \tag{35}$$

Equation (30) is solved iteratively at each loop k. Some of our results with such linear or non linear method can be seen in [4] or [2], more specifically [1] is a custom implementation of the Levenberg-Marquardt algorithm based on the adjoint method (developed by Jacques Louis Lions in 1968) coupled to the conjugate gradient algorithm to estimate wide properties field in a medium.

3.3. Reflectometry-based methods for electrical engineering and for civil engineering

The fast development of electronic devices in modern engineering systems involves more and more connections through cables, and consequently, with an increasing number of connection failures. Wires and connectors are subject to ageing and degradation, sometimes under severe environmental conditions. In many applications, the reliability of electrical connexions is related to the quality of production or service, whereas in critical applications reliability becomes also a safety issue. It is thus important to design smart diagnosis systems able to detect connection defects in real time. This fact has motivated research projects on methods for fault diagnosis in this field. Some of these projects are based on techniques of reflectometry, which consist in injecting waves into a cable or a network and in analyzing the reflections. Depending on the injected waveforms and on the methods of analysis, various techniques of reflectometry are available. They all have the common advantage of being non destructive.

At Inria the research activities on reflectometry started within the SISYPHE EPI several years ago and now continue in the I4S EPI. Our most notable contribution in this area is a method based on the *inverse scattering* theory for the computation of *distributed characteristic impedance* along a cable from reflectometry measurements [14], [11], [56]. It provides an efficient solution for the diagnosis of *soft* faults in electrical cables, like in the example illustrated in Figure 3 . While most reflectometry methods for fault diagnosis are based on the detection and localization of impedance discontinuity, our method yielding the spatial profile of the characteristic impedance is particularly suitable for the diagnosis of soft faults *with no or weak impedance discontinuities*.

Fault diagnosis for wired networks have also been studied in Inria [58], [54]. The main results concern, on the one hand, simple star-shaped networks from measurements made at a single node, on the other hand, complex networks of arbitrary topological structure with complete node observations.

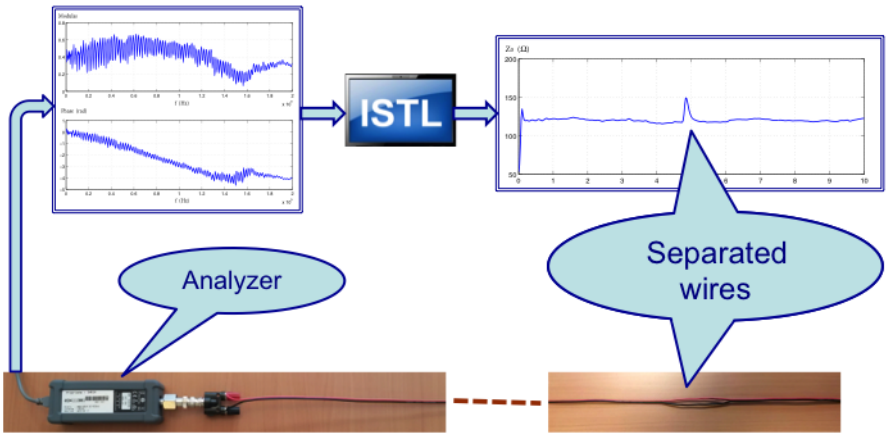

Figure 3. Inverse scattering software (ISTL) for cable soft fault diagnosis.

Though initially our studies on reflectometry were aiming at applications in electrical engineering, since the creation of the I4S team, we are also investigating applications in the field of civil engineering, by using electrical cables as sensors for monitoring changes in mechanical structures.

What follows is about some basic elements on mathematical equations of electric cables and networks, the main approach we follow in our study, and our future research directions.

3.3.1. Mathematical model of electric cables and networks

A cable excited by a signal generator can be characterized by the telegrapher's equations [55]

$$\begin{aligned} &\frac{\partial}{\partial z}V(t,z) + L(z)\frac{\partial}{\partial t}I(t,z) + R(z)I(t,z) = 0 \\ &\frac{\partial}{\partial z}I(t,z) + C(z)\frac{\partial}{\partial t}V(t,z) + G(z)V(t,z) = 0 \end{aligned} \tag{36}$$

where t represents the time, z is the longitudinal coordinate along the cable, $V(t,z)$ and $I(t,z)$ are respectively the voltage and the current in the cable at the time instant t and at the position z, $R(z), L(z), C(z)$ and $G(z)$ denote respectively the series resistance, the inductance, the capacitance and the shunt conductance per unit length of the cable at the position z. The left end of the cable (corresponding to $z = a$) is connected to a voltage source $V_s(t)$ with internal impedance R_s. The quantities $V_s(t)$, R_s, $V(t,a)$ and $I(t,a)$ are related by

$$V(t,a) = V_s(t) - R_s I(t,a). \tag{37}$$

At the right end of the cable (corresponding to $z = b$), the cable is connected to a load of impedance R_L, such that

$$V(t,b) \quad = R_L I(t,b). \tag{38}$$

One way for deriving the above model is to spatially discretize the cable and to characterize each small segment with 4 basic lumped parameter elements for the j-th segment: a resistance ΔR_j, an inductance ΔL_j, a capacitance ΔC_j and a conductance ΔG_j. The entire circuit is described by a system of ordinary differential equations. When the spatial discretization step size tends to zero, the limiting model leads to the telegrapher's equations.

A wired network is a set of cables connected at some nodes, where loads and sources can also be connected. Within each cable the current and voltage satisfy the telegrapher's equations, whereas at each node the current and voltage satisfy the Kirchhoff's laws, unless in case of connector failures.

3.3.2. The inverse scattering theory applied to cables

The inverse scattering transform was developed during the 1970s-1980s for the analysis of some nonlinear partial differential equations [53]. The visionary idea of applying this theory to solving the cable inverse problem goes also back to the 1980s [52]. After having completed some theoretic results directly linked to practice [14], [56], we started to successfully apply the inverse scattering theory to cable soft fault diagnosis, in collaboration with GEEPS-SUPELEC [11].

To link electric cables to the inverse scattering theory, the telegrapher's equations are transformed in a few steps to fit into a particular form studied in the inverse scattering theory. The Fourier transform is first applied to obtain a frequency domain model, the spatial coordinate z is then replaced by the propagation time

$$x(z) = \int_0^z \sqrt{L(s)C(s)}ds$$

and the frequency domain variables $V(\omega,x), I(\omega,x)$ are replaced by the pair

$$\begin{aligned} \nu_1(\omega,x) &= \frac{1}{2}\left[Z_0^{-\frac{1}{2}}(x)U(\omega,x) - Z_0^{\frac{1}{2}}(x)I(\omega,x)\right] \\ \nu_2(\omega,x) &= \frac{1}{2}\left[Z_0^{-\frac{1}{2}}(x)U(\omega,x) + Z_0^{\frac{1}{2}}(x)I(\omega,x)\right] \end{aligned} \tag{39}$$

with

$$Z_0(x) = \sqrt{\frac{L(x)}{C(x)}}. \tag{40}$$

These transformations lead to the Zakharov-Shabat equations

$$\begin{aligned} \frac{d\nu_1(\omega,x)}{dx} + ik\nu_1(\omega,x) &= q^*(x)\nu_1(\omega,x) + q^+(x)\nu_2(\omega,x) \\ \frac{d\nu_2(\omega,x)}{dx} - ik\nu_2(\omega,x) &= q^-(x)\nu_1(\omega,x) - q^*(x)\nu_2(\omega,x) \end{aligned} \tag{41}$$

with

$$\begin{aligned} q^{\pm}(x) &= -\frac{1}{4}\frac{d}{dx}\left[ln\frac{L(x)}{C(x)}\right] \mp \frac{1}{2}\left[\frac{R(x)}{L(x)} - \frac{G(x)}{C(x)}\right] \\ &= -\frac{1}{2Z_0(x)}\frac{d}{dx}Z_0(x) \mp \frac{1}{2}\left[\frac{R(x)}{L(x)} - \frac{G(x)}{C(x)}\right] \\ q^{*}(x) &= \frac{1}{2}\left[\frac{R(x)}{L(x)} + \frac{G(x)}{C(x)}\right]. \end{aligned} \tag{42}$$

These equations have been well studied in the inverse scattering theory, for the purpose of determining partly the "potential functions" $q^{\pm}(x)$ and $q^{*}(x)$ from the scattering data matrix, which turns out to correspond to the data typically collected with reflectometry instruments. For instance, it is possible to compute the function $Z_0(x)$ defined in (35), often known as the characteristic impedance, from the reflection coefficient measured at one end of the cable. Such an example is illustrated in Figure 3 . Any fault affecting the characteristic impedance, like in the example of Figure 3 caused by a slight geometric deformation, can thus be efficiently detected, localized and characterized.

3.4. Research Program

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

3.4.1. Vibration analysis and monitoring

3.4.1.1. Direct vibration modeling under temperature changes

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

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

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

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

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

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

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

3.4.1.3. Uncertainty quantification for system identification algorithms

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

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

The inverse scattering method we developed is efficient for the diagnosis of all soft faults affecting the characteristic impedance, the major parameter of a cable. In some particular applications, however, faults would rather affect the series resistance (ohmic loss) or shunt conductance (leakage loss) than the characteristic impedance. The first method we developed for the diagnosis of such losses had some numerical stability problems. The new method is much more reliable and efficient. It is also important to develop efficient solutions for long cables, up to a few kilometers.

For wired networks, the methods we already developed cover either the case of simple networks with a single node measurement or the case of complex networks with complete node measurements. Further developments are still necessary for intermediate situations.

In terms of applications, the use of electric cables as sensors for the monitoring of various structures is still at its beginning. We believe that this new technology has a strong potential in different fields, notably in civil engineering and in materials engineering.

3.4.3. Non Destructive testing of CFRP bonded on concrete through active thermography

Strengthening or retrofitting of reinforced concrete structures by externally bonded fiber-reinforced polymer (FRP) systems is now a commonly accepted and widespread technique. However, the use of bonding techniques always implies following rigorous installation procedures. The number of carbon fiber-reinforced polymer (CFRP) sheets and the glue layer thickness are designed by civil engineers to address strengthening objectives. Moreover, professional crews have to be trained accordingly in order to ensure the durability and long-term performance of the FRP reinforcements. Conformity checking through an ‘in situ’ verification of the bonded FRP systems is then highly desirable. The quality control programme should involve a set of adequate inspections and tests. Visual inspection and acoustic sounding (hammer tap) are commonly used to detect delaminations (disbonds). Nevertheless, these techniques are unable to provide sufficient information about the depth (in case of multilayered composite) and width of the disbonded areas. They are also incapable of evaluating the degree of adhesion between the FRP and the substrate (partial delamination, damage of the resin and poor mechanical properties of the resin). Consequently, rapid and efficient inspection methods are required. Among the non-destructive (NDT) methods currently under study, active infrared thermography is investigated due to its ability to be used in the field. In such context and to reach the aim of having an in situ efficient NDT method, we carried out experiments and subsequent data analysis using thermal excitation. Image processing, inverse thermal modelling and 3D numerical simulations are used and then applied to experimental data obtained in laboratory conditions.

3.4.4. IRSHM: Multi-Sensing system for outdoor thermal monitoring

Ageing of transport infrastructures combined with traffic and climatic solicitations contribute to the reduction of their performances. To address and quantify the resilience of civil engineering structure, investigations on robust, fast and efficient methods are required. Among research works carried out at IFSTTAR, methods for long term monitoring face an increasing demand. Such works take benefits of this last decade technological progresses in ICT domain.

Thanks to IFSTTAR years of experience in large scale civil engineering experiment, I4S is able to perform very long term thermal monitoring of structures exposed to environmental condition, as the solar heat flux, natural convection or seasonal perturbation. Informations system are developed to asses the data acquisition and researchers work on the quantification of the data to detect flaws emergence on structure, those techniques are also used to diagnose thermal insulation of buildings or monitoring of guided transport infrastructures, Figure 4 left. Experiments are carried out on a real transport infrastructure open to traffic and buildings. The detection of the inner structure of the deck is achieved by image processing techniques (as FFT), principal component thermography (PCT), Figure 4 right, or characterization of the inner structure thanks to an original image processing approach.

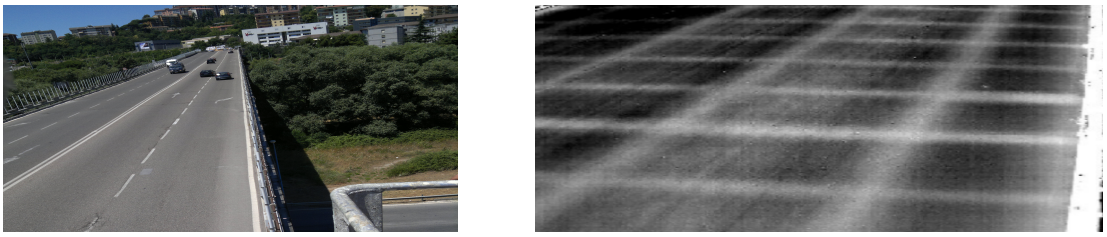

Figure 4. Left: Image in the visible spectrum of the deck surface - Right: PCT result on a bridge deck

For the next few years, I4S is actively implied in the SenseCity EQUIPEX (http://sense-city.ifsttar.fr/) where our informations systems are used to monitor a mini-city replica, Figure 5 .

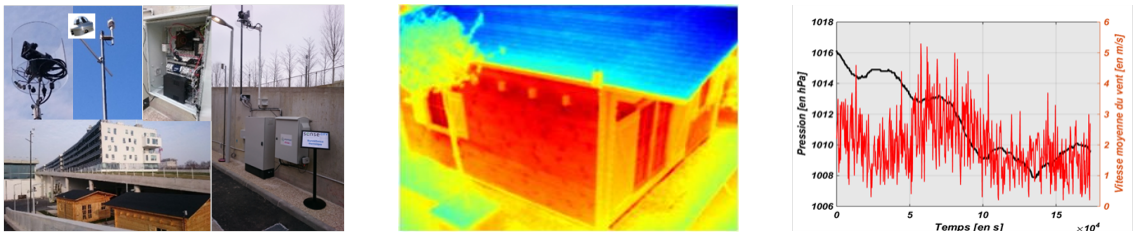

Figure 5. Various view and results of the SenseCity experimentation site - (site and hardware view, IR imaging, Environmental Monitoring)

3.4.5. R5G: The 5th Generation Road

The road has to reinvent itself periodically in response to innovations, societal issues and rising user expectations. The 5th Generation Road (R5G) focuses firmly on the future and sets out to be automated, safe, sustainable and suited to travel needs. Several research teams are involved in work related to this flagship

project for IFSTTAR, which is a stakeholder in the Forever Open Road. Through its partnership with the COSYS (IFSTTAR) department, I4S is fully involved in the development of the 5th Generation Road.

Most of the innovations featured in R5G are now mature, for example communication and few solutions for energy exchange between the infrastructure, the vehicle and the network manager; recyclable materials with the potential for self-diagnosis and repair, a pavement surface that remains permanently optimal irrespective of climatic variations… Nevertheless, implementing them on an industrial scale at a reasonable cost still represents a real challenge. Consultation with the stakeholders (researchers, industry, road network owners and users) has already established the priorities for the creation of full-scale demonstrators. The next stages are to achieve synergy between the technologies tested by the demonstrators, to manage the interfaces and get society to adopt R5G.

MCTAO Project-Team

3. Research Program

3.1. Control Problems

McTAO's major field of expertise is control theory in the large. Let us give an overview of this field.

Modelling. Our effort is directed toward efficient methods for the control of real (physical) *systems*, based on a *model* of the system to be controlled. Choosing accurate models yet simple enough to allow control design is in itself a key issue. The typical continuous-time model is of the form $\mathrm{d}x/\mathrm{d}t = f(x,u)$ where x is the *state*, ideally finite dimensional, and u the *control*; the control is left free to be a function of time, or a function of the state, or obtained as the solution of another dynamical system that takes x as an input. Modelling amounts to deciding the nature and dimension of x, as well as the dynamics (roughly speaking the function f). Connected to modeling is identification of parameters when a finite number of parameters are left free in "f".

Controllability, path planning. Controllability is a property of a control system (in fact of a model) that two states in the state space can be connected by a trajectory generated by some control, here taken as an explicit function of time. Deciding on local or global controllability is still a difficult open question in general. In most cases, controllability can be decided by linear approximation, or non-controllability by "physical" first integrals that the control does not affect. For some critically actuated systems, it is still difficult to decide local or global controllability, and the general problem is anyway still open.

Path planning is the problem of constructing the control that actually steers one state to another.

Optimal control. In optimal control, one wants to find, among the controls that satisfy some contraints at initial and final time (for instance given initial and final state as in path planning), the ones that minimize some criterion.
This is important in many control engineering problems, because minimizing a cost is often very relevant. Mathematically speaking, optimal control is the modern branch of the calculus of variations, rather well established and mature [70], [47], [37], but with a lot of hard open questions. In the end, in order to actually compute these controls, ad-hoc numerical schemes have to be derived for effective computations of the optimal solutions.
See more about our research program in optimal control in section 3.2 .

Feedback control. In the above two paragraphs, the control is an explicit function of time. To address in particular the stability issues (sensitivity to errors in the model or the initial conditions for example), the control has to be taken as a function of the (measured) state, or part of it. This is known as closed-loop control; it must be combined with optimal control in many real problems.

On the problem of stabilization, there is longstanding research record from members of the team, in particular on the construction of "Control Lyapunov Functions", see [61], [72].

Classification of control systems One may perform various classes of transformations acting on systems, or rather on models... The simpler ones come from point-to-point transformations (changes of variables) on the state and control, and more intricate ones consist in embedding an extraneous dynamical system into the model, these are dynamic feedback transformations, they change the dimension of the state.

In most problems, choosing the proper coordinates, or the right quantities that describe a phenomenon, sheds light on a path to the solution; these proper choices may sometimes be found from an understanding of the modelled phenomenons, or it can come from the study of the geometry of the equations and the transformation acting on them. This justifies the investigations of these transformations on models for themselves.

These topics are central in control theory; they are present in the team, see for instance the classification aspect in [52] or —although this research has not been active very recently— the study [69] of dynamic feedback and the so-called "flatness" property [64].

3.2. Optimal Control and its Geometry

Let us detail our research program concerning optimal control. Relying on Hamiltonian dynamics is now prevalent, instead of the Lagrangian formalism in classical calculus of variations. The two points of view run parallel when computing geodesics and shortest path in Riemannian Geometry for instance, in that there is a clear one-to-one correspondance between the solutions of the geodesic equation in the tangent bundle and the solution of the Pontryagin Maximum Principle in the cotangent bundle. In most optimal control problems, on the contrary, due to the differential constraints (velocities of feasible trajectories do not cover all directions in the state space), the Lagrangian formalism becomes more involved, while the Pontryagin Maximum Principle keeps the same form, its solutions still live in the cotangent bundle, their projections are the extremals, and a minimizing curve must be the projection of such a solution.

Cut and conjugate loci. The cut locus —made of the points where the extremals lose optimality— is obviously crucial in optimal control, but usually out of reach (even in low dimensions), and anyway does not have an analytic characterization because it is a non-local object. Fortunately, conjugate points —where the extremals lose *local* optimality— can be effectively computed with high accuracy for many control systems. Elaborating on the seminal work of the Russian and French schools (see [74], [38], [39] and [53] among others), efficient algorithms were designed to treat the smooth case. This was the starting point of a series of papers of members of the team culminating in the outcome of the *cotcot* software [46], followed by the *Hampath* [55] code. Over the years, these codes have allowed for the computation of conjugate loci in a wealth of situations including applications to space mechanics, quantum control, and more recently swimming at low Reynolds number.

With in mind the two-dimensional analytic Riemannian framework, a heuristic approach to the global issue of determining cut points is to search for singularities of the conjugate loci; this line is however very delicate to follow on problems stemming from applications in three or more dimensions (see *e.g.* [56] and [43]).

Recently, computation of conjugate points was conducted in [6], [5] to determine the optimality status in swimming at low Reynolds number; because of symmetries, and of the periodicity constraint, a tailor-made notion of conjugate point had to be used, see more in [65]. In all these situations, the fundamental object underlying the analysis is the curvature tensor. In Hamiltonian terms, one considers the dynamics of subspaces (spanned by Jacobi fields) in the Lagrangian Grassmannian [36]. This point of view withstands generalizations far beyond the smooth case: In L^1-minimization, for instance, discontinuous curves in the Grassmannian have to be considered (instantaneous rotations of Lagrangian subspaces still obeying symplectic rules [60]).

The cut locus is a central object in Riemannian geometry, control and optimal transport. This is the motivation for a series of conferences on "The cut locus: A bridge over differential geometry, optimal control, and transport", co-organized by team members and Japanese colleagues, see section 10.1.1 .

Riemann and Finsler geometry. Studying the distance and minimising geodesics in Riemannian Geometry or Finsler Geometry is a particular case of optimal control, simpler because there are no differential constraints; it is studied in the team for the following two reasons. On the one hand, after some tranformations, like averaging (see section 3.2) or reduction, some more difficult optimal control problems lead to a Riemann or Finsler geometry problem. On the other hand, optimal control, mostly the Hamiltonian setting, brings a fresh viewpoint on problems in Riemann and Finsler geometry.

On Riemannian ellipsoids of revolution, the optimal control approach allowed to decide on the convexity of the injectivity domain, which, associated with non-negativity of the Ma-Trudinger-Wang curvature tensor, ensures continuity of the optimal transport on the ambient Riemannian manifold [63], [62]. The analysis in the oblate geometry [44] was completed in [59] in the prolate one, including a preliminary analysis of non-focal domains associated with conjugate loci.

Averaging in systems coming from space mechanics control (see sections 3.2 and 4.1) with L^2-minimization yields a Riemannian metric, thoroughly computed in [42] together with its geodesic flow; in reduced dimension, its conjugate and cut loci were computed in [45] with Japanese Riemannian geometers. Averaging the same systems for minimum time yields a Finsler Metric, as noted in [41]. In [51], the geodesic convexity properties of these two types of metrics were compared. When perturbations (other than the control) are considered, they introduce a "drift", *i.e.* the Finsler metric is no longer symmetric.

Sub-Riemannian Geometry. Optimal control problems that pertain to sub-Riemannian Geometry bear all the difficulties of optimal control, like the role of singular/abnormal trajectories, while having some useful structure. They lead to many open problems, like smoothness of minimisers, see the recent monograph [68] for an introduction. Let us detail one open question related to these singular trajectories: the Sard conjecture in sub-Riemannian geometry.

Given a totally non-holonomic distribution on a smooth manifold, the Sard Conjecture is concerned with the size of the set of points that can be reached by singular horizontal paths starting from a given point. In the setting of rank-two distributions in dimension three, the Sard conjecture is that this set should be a subset of the so-called Martinet surface, indeed small both in measure and in dimension. In [4], it has been proved that the conjecture holds in the case where the Martinet surface is smooth. Moreover, the case of singular real-analytic Martinet surfaces was also addressed. In this case, it was shown that the Sard Conjecture holds true under an assumption of non-transversality of the distribution on the singular set of the Martinet surface. It is, of course, very intersting to get rid of the remaining technical assumption, or to go to higher dimension. Note that any Sard-type result has strong consequences on the regularity of sub-Riemannian distance functions and in turn on optimal transport problems in the sub-Riemannian setting.

Small controls and conservative systems, averaging. Using averaging techniques to study small perturbations of integrable Hamiltonian systems is as old an idea as celestial mechanics. 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 [40], [73].

This line of research stemmed out of applications to space engineering (see section 4.1): the control of the super-integrable Keplerian motion of a spacecraft orbiting around the Earth is an example of a slow-fast controlled system. Since weak propulsion is used, the control itself acts as a perturbation, among other perturbations of similar magnitudes: higher order terms of the Earth potential (including J_2 effect, first), potential of more distant celestial bodies (such as the Sun and the Moon), atmospheric drag, or even radiation pressure.

Properly qualifying the convergence properties (when the small parameter goes to zero) is important and is made difficult by the presence of control. In [41], convergence is seen as convergence to a differential inclusion; this applies to minimum time; a contribution of this work is to put forward the metric character of the averaged system by yielding a Finsler metric (see section 3.2). Proving convergence of the extremals (solutions of the Pontryagin Maximum Principle) is more intricate. In [58], standard averaging ([40], [73]) is performed on the minimum time extremal flow after carefully identifying slow variables of the system thanks to a symplectic reduction. This alternative approach allows to retrieve the previous metric approximation, and to partly address the question of convergence. Under suitable assumptions on a given geodesic of the averaged system (disconjugacy conditions, namely), one proves existence of a family of quasi-extremals for the original system that converge towards the geodesic when the small perturbation parameter goes to zero. This needs to be improved, but convergence of all extremals to extremals of an "averaged Pontryagin Maximum Principle" certainly fails. In particular, one cannot hope for C^1-regularity on the value function when the small parameter goes to zero as swallowtail-like singularities due to the structure of local minima in the problem are expected. (A preliminary analysis has been made in [57].)

Optimality of periodic solutions/periodic controls. When seeking to minimize a cost with the constraint that the controls and/or part of the states are periodic (and with other initial and final conditions), the notion of conjugate points is more difficult than with straightforward fixed initial point. In [48], for the problem of optimizing the efficiency of the displacement of some micro-swimmers (see section 4.3) with periodic deformations, we used the sufficient optimality conditions established by R. Vinter's group [78], [65] for systems with non unique minimizers due to the existence of a group of symmetry (always present with a periodic minimizer-candidate control). This takes place in a long term collaboration with P. Bettiol (Univ. Bretagne Ouest) on second order sufficient optimality conditions for periodic solutions, or in the presence of higher dimensional symmetry groups, following [78], [65].

Another question relevant to locomotion is the following. Observing animals (or humans), or numerically solving the optimal control problem associated with driftless micro-swimmers for various initial and final conditions, we remark that the optimal strategies of deformation seem to be periodic, at least asymptotically for large distances. This observation is the starting point for characterizing dynamics for which some optimal solutions are periodic, and asymptotically attract other solutions as the final time grows large; this is reminiscent of the "turnpike theorem" (classical, recently applied to nonlinear situations in [77]).

Software. These applications (but also the development of theory where numerical experiments can be very enlightening) require many algorithmic and numerical developments that are an important side of the team activity. The software *Hampath* (see section 6.1) is maintained by former members of the team in close collaboration with McTAO. We also use direct discretization approaches (such as the Bocop solver developed by COMMANDS) in parallel. Apart from this, we develop on-demand algorithms and pieces of software, for instance we have to interact with a production software developed by Thales Alenia Space. A strong asset of the team is the interplay of its expertise in geometric control theory with applications and algorithms (see sections 4.1 to 4.3) on one hand, and with optimal transport, and more recently Hamiltonian dynamics, on the other.

3.3. Optimal Transport

Given two measures, and calling transport maps the maps that transport the first measure into the second one, the Monge-Kantorovich problem of Optimal Transport is the search of the minimum of some cost on the set of transport maps. The cost of a map usually comes from some point to point cost and the transport measure. This topic attracted renewed attention in the last decade, and has ongoing applications of many types. Matching optimal transport with geometric control theory is one originality of our team.

Let us sketch an important class of open problems. In collaboration with R. McCann [67], we worked towards identifying the costs that admit unique optimizers in the Monge-Kantorovich problem of optimal transport between arbitrary probability densities. For smooth costs and densities on compact manifolds, the only known examples for which the optimal solution is always unique require at least one of the two underlying spaces to be homeomorphic to a sphere. We have introduced a multivalued dynamics induced by the transportation cost between the target and source space, for which the presence or absence of a sufficiently large set of periodic trajectories plays a role in determining whether or not optimal transport is necessarily unique. This insight allows us to construct smooth costs on a pair of compact manifolds with arbitrary topology, so that the optimal transport between any pair of probability densities is unique. We investigated further this problem of uniquely minimizing costs and obtained in collaboration with Abbas Moameni [12] a result of density of uniquely minimizing costs in the C^0-topology. The results in higher topology should be the subject of some further research.

NECS Project-Team

3. Research Program

3.1. Introduction

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

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

3.2. Distributed estimation and data fusion in network systems

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

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

3.3. Network systems and graph analysis

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

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

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

3.4. Collaborative and distributed network control

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

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

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

3.5. Transportation networks

This is currently the main application domain of the NECS team. Several interesting problems in this area capture many of the generic networks problems identified before (e.g., decentralized/collaborative traffic optimal control, density balancing using consensus concepts, data fusion, distributed estimation, etc.). Several specific actions have been continued/launched to this purpose: improvement and finalization of the Grenoble Traffic Lab(GTL), EU projects (SPEEDD, ERC-AdG Scale-FreeBack). Further research goals are envisioned, such as:

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

NON-A POST Team

3. Research Program

3.1. Theory of homogeneous systems

Homogeneity is a property of mathematical objects, such as functions or vector fields, to be scaled in a consistent manner with respect to a scaling operation (called a dilation) applied to their argument (a kind of symmetry). The first rise of homogeneity deals with homogeneous polynomials investigated by L. Euler in 18^{th} century. In 50s and 60s more generic notions of homogeneity (weighted and coordinate-free or geometric) have been introduced by V.I. Zubov and his group. For example, a function $f : \mathbb{R}^n \to \mathbb{R}$ is called homogeneous (in Euler's sense) if

$$f(\lambda x) = \lambda^{1+\nu} f(x) \quad \forall x \in \mathbb{R}^n,\ \forall \lambda > 0$$

for some $\nu \geq -1$ called the degree of homogeneity of f (a parameter of symmetry). Such a type of symmetry leads to the scaling of trajectories of resultant dynamical systems, *e.g.* for

$$\dot{x}(t) = f\left(x(t)\right) \quad t \geq 0,\ x(0) = x_0 \in \mathbb{R}^n$$

denote a solution corresponding to the initial condition x_0 by $X(t, x_0)$, then

$$X(t, \lambda x_0) = \lambda X(\lambda^{\nu} t, x_0) \quad \forall x_0 \in \mathbb{R}^n,\ \forall \lambda > 0.$$

So homogeneous systems possess several important and useful properties: their local behavior is the same as global one, the rate of convergence to the origin can be identified by degree of homogeneity, the stability is robust to various perturbations. There are also plenty of researches performed in the last 30 years and the members of *Non-A POST* team extended these notions of homogeneity to discontinuous systems (in a geometric framework), time-delay systems, partial differential equations, time-varying systems, and recently to discrete-time models (together with the concept of local homogeneity). They also proposed plenty of control and estimation algorithms based on homogeneity.

Advantages of homogeneous algorithms taking into account the above mentioned criteria:

A1) The rate of convergence in homogeneous systems can be qualified by its degree (finite-time and fixed-time for negative and positive degrees, respectively).

A2) Due to symmetry of these systems they admit special discretization tools (also developed by the members of *Non-A POST* team), which make simpler they realization for on-line scenarios.

A3) The internal symmetry of these dynamics makes them inherently robust with respect to external perturbations, measurement noises and delays, which is especially important in networked systems.

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 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* and *Non-A* teams, which rely on the only information contained in the output signal and its derivatives.

3.3. FT and FxT control and estimation

To design an estimation or control algorithm we have to select a performance criterion to be optimized. Stability is one of the main performance indexes, which has to be established during analysis or design of a dynamical system. Stability is usually investigated with respect to an invariant mode (*e.g.*, an equilibrium, desired trajectory or a limit cycle), then another important characteristics is the time of convergence of the system trajectories to this mode, which can be *asymptotic* (in conventional approaches) or *finite-time* (being the focus of *Non-A POST* team). In the latter case the limit mode has to be exactly established in a finite time dependent on initial deviations (if such a time is independent on initial conditions, then this type of convergence is called *fixed-time*). If the rate of convergence is just faster than any exponential of time, then such a convergence is called *hyperexponential*. The notion of finite-time stability has been proposed in 60s by E. Roxin and it has been developed in many works later, where a particular attention is paid to the time of convergence for trajectories to a steady state (it is worth to note that there exists another notion having the same name, *i.e.* finite-time or short-time stability, which is focused on analysis of a dynamical system behavior on bounded intervals of time, and it is completely different and not considered here). For example, the following simple scalar dynamics:

$$\dot{x}(t) = -|x(t)|^{1+\nu}\text{sign}(x(t)) \quad \forall t \geq 0,\ x(t) \in \mathbb{R},$$

has the solution $x(t) = \beta(|x_0|, t)\text{sign}(x_0)$ for any initial condition $x(0) = x_0 \in \mathbb{R}$, where

$$\beta(s,t) = \begin{cases} \begin{cases} \left(s^{-\nu} + \nu t\right)^{-\frac{1}{\nu}} & t < -\frac{s^{-\nu}}{\nu} \\ 0 & t \geq -\frac{s^{-\nu}}{\nu} \end{cases} & -1 \leq \nu < 0 \\ \mathrm{e}^{-t}s & \nu = 0 \\ \frac{s}{(1+\nu s^{\nu} t)^{\frac{1}{\nu}}} & \nu > 0 \end{cases},$$

which possesses a finite-time convergence with the settling time $-\frac{|x_0|^{-\nu}}{\nu}$ for $-1 \leq \nu < 0$, an exponential convergence for $\nu = 0$ and the fixed time of convergence to the unit ball is bounded by ν^{-1} for $\nu > 0$. It is straightforward to check that this simple system is homogeneous of degree ν. The members of *Non-A POST* team obtained many results on analysis and design of control and estimation algorithms in this context. A useful and simple method to deal with these three types of convergence (finite-time, fixed-time or hyperexponential) is based on the theory of *homogeneous* systems.

[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").

[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.

3.4. Applications

The application of the developed control and estimation algorithms for different scenarios in IoT is a priority for *Non-A POST* team. Participation in different potential applications allows the team to better understand the features of IoT and their required performances. A list of possible applications, partially already addressed in the team, is as follows:

- smart bivalve-based biosensor for water quality monitoring (ANR project WaQMoS): presence of persistent external perturbations, which are hard to measure, and important model uncertainty make application of conventional techniques complicated; another issue is consensus seeking between animals for a contamination detection;
- control and estimation for flying vehicles, *e.g.* quadrotors or blimps (1 PhD ONERA, 2 PhDs EC Lille): nonlinearity of the model and its uncertainty coupled with important aerodynamic perturbations have to be compensated by fast (finite- or fixed-time) and robust control and estimation algorithms;
- human behavior modeling and estimation with posterior design of algorithms for human-computer interaction (ANR project TurboTouch): robust finite-time differentiators demonstrate good estimation capabilities needed for prediction in this application;
- human physiological characteristics estimation (like emotion detection, galvanic skin response filtering, fatigue evaluation in collaborations with Neotrope and Ellcie Healthy): intelligent robust filtering and finite-time distributed estimation are key features in this scenario;
- path planning for autonomous vehicles taking into account behavior of humans (PhD CIFRE with SEQUEL team and Renault): application of interval estimation and prediction techniques to treat the uncertainty of the environment by reducing computational complexity of reinforcement learning;
- flow control (in the framework of ContrATech subprogram of CPER ELSAT): the case of control and estimation of a distributed-parameter system with very fast and uncertain dynamics, where finite-time solutions developed by *Non-A POST* team are necessary

Involvement in various real-world scenarios will allow *Non-A POST* to develop demonstrators of disposed technologies with application to IoT.

QUANTIC Project-Team

3. Research Program

3.1. Hardware-efficient quantum information processing

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

The usual approach for the realization of QEC is to use many qubits to obtain a larger Hilbert space of the qubit register [85], [88]. 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 [62]. 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 [59], [53] 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 [61]. Through a recent experimental work [93], we benefit from this controllability to prepare superpositions of quasi-orthogonal coherent states, also known as Schrödinger cat states.

In this Scheme, the logical qubit is encoded in a four-component Schrödinger cat state. Continuous quantum non-demolition (QND) monitoring of a single physical observable, consisting of photon number parity, enables then the tractability of single photon jumps. We obtain therefore a first-order quantum error correcting code using only a single high-Q cavity mode (for the storage of quantum information), a single qubit (providing the non-linearity needed for controllability) and a single low-Q cavity mode (for reading out the error syndrome).

An earlier experiment on such QND photon-number parity measurements [89] has recently led to a first experimental realization of a full quantum error correcting code improving the coherence time of quantum information [5]. 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.

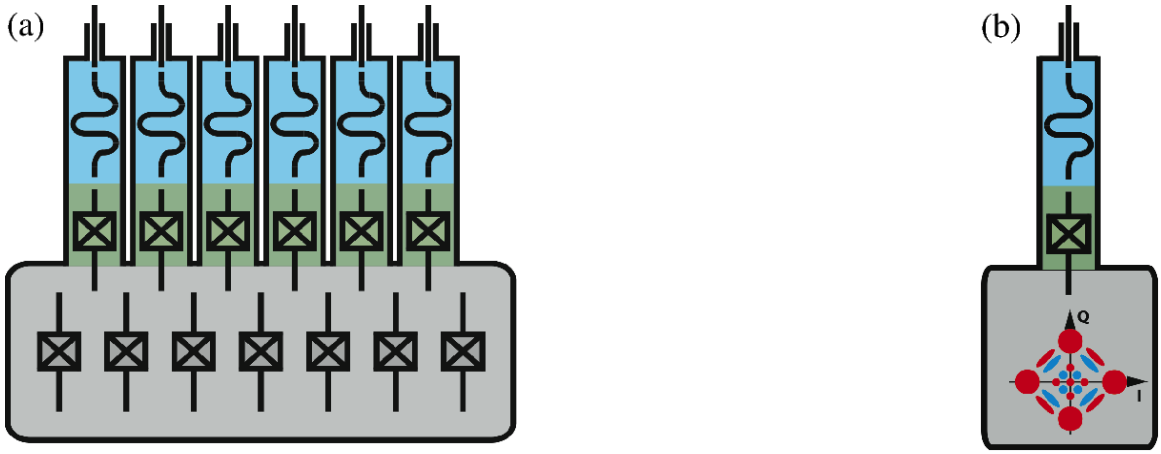

Figure 1. (a) A protected logical qubit consisting of a register of many qubits: here, we see a possible architecture for the Steane code [88] consisting of 7 qubits requiring the measurement of 6 error syndromes. In this sketch, 7 transmon qubits in a high-Q resonator and the measurement of the 6 error syndromes is ensured through 6 additional ancillary qubits with the possibility of individual readout of the ancillary qubits via independent low-Q resonators. (b) Minimal architecture for a protected logical qubit, adapted to circuit quantum electrodynamics experiments. Quantum information is encoded in a Schrödinger cat state of a single high-Q resonator mode and a single error syndrome is measured, using a single ancillary transmon qubit and the associated readout low-Q resonator.

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 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-demolition* (QND) measurement has played a crucial role in understanding and resolving this difficulty [36]. In the context of cavity quantum electro-dynamics (cavity QED) with Rydberg atoms [55], a first experiment on continuous QND measurements of the number of microwave photons was performed by the group at Laboratoire Kastler-Brossel (ENS) [54]. Later on, this ability of performing continuous measurements allowed the same group to realize the first continuous quantum feedback protocol stabilizing highly non-classical states of the microwave field in the cavity, the so-called photon number states [8] (this ground-breaking work was mentioned in the Nobel prize attributed to Serge Haroche). The QUANTIC team contributed to the theoretical work behind this experiment [45], [27], [87], [29]. 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) [44], recent advances in quantum-limited amplifiers [79], [91] have opened doors to high-fidelity non-demolition measurements and real-time feedback for superconducting qubits [56]. 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 [91], [78], [38]. Here again, the QUANTIC team has participated to one of the first experiments in the field where the control objective is to track a dynamical trajectory of a single qubit rather than stabilizing a stationary state. Such quantum trajectory tracking could be further explored to achieve metrological goals such as the stabilization of the amplitude of a microwave drive [69].

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 [76] and the closely related coherent feedback [67] 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 [52], single-qubit state stabilization [71], and the creation [31] and stabilization [60], [66][9] of states of multipartite quantum systems.

Such reservoir engineering techniques could be widely revisited exploring the flexibility in the Hamiltonian design for QSC. We have recently developed theoretical proposals leading to extremely efficient, and simple to implement, stabilization schemes for systems consisting of a single, two or three qubits [52], [64], [42][12]. The experimental results based on these protocols have illustrated the efficiency of the approach [52][9]. Through these experiments, we exploit the strong dispersive interaction [83] between superconducting qubits and a single low-Q cavity mode playing the role of a dissipative reservoir. Applying continuous-wave (cw) microwave drives with well-chosen fixed frequencies, amplitudes, and phases, we engineer an effective interaction Hamiltonian which evacuates the entropy of the system interacting with a noisy environment: by driving the qubits and cavity with continuous-wave drives, we induce an autonomous feedback loop which corrects the state of the qubits every time it decays out of the desired target state. The schemes are robust against small variations of the control parameters (drives amplitudes and phase) and require only some basic calibration. Finally, by avoiding resonant interactions between the qubits and the low-Q cavity mode, the qubits remain protected against the Purcell effect, which would reduce the coherence times. We have also investigated both theoretically and experimentally the autonomous stabilization of non-classical states (such as Schrodinger cat states and Fock states) of microwave field confined in a high-Q cavity mode [70], [81], [57][4].

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 [80], [27], [86], [82], [87], [29][7] 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 [29]: 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 [94]; 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 [74]. 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 [56], [38].

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 [32] and is related to quantum trajectories [40], [43]. A modern and mathematical exposure of the diffusive models is given in [30]. In [95] 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 [80], [86]. This stability result is extended to a large class of continuous-time filters in [28]. Further efforts are required to characterize asymptotic and exponential stability. Estimations of convergence rates are available only for quantum non-demolition measurements [33]. Parameter estimations based on measurement data of quantum trajectories can be formulated within such quantum filtering framework [47], [72].

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 [37] that post-selection statistics and "past quantum" state analysis [48] 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 [76], [67]. The closed-loop system is then a composite system built with the original system and its controller. In fact, and given our particular recent expertise in this domain [7], [9] [52], 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 [75]). 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., [26][chapter 4, section 6]). When the goal steady-state is not full rank very few convergence results are available.

We will focus on this geometric situation where the goal steady-state is on the boundary of the cone of positive Hermitian operators of finite trace. A specific attention will be given to adapt standard tools (Lyapunov function, passivity, contraction and Lasalle's invariance principle) for infinite dimensional systems to spin/spring structures inspired of [7], [9] [52], [70] 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 [51], [50]. We will start with [84] and [77] where, based on a theorem due to Birkhoff [34], 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 [90] and by our recent generalized extension of the latter synchronizing interactions to quantum systems [68].

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 [73], 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 [92], [65] with experimental limitations. The characterization of Kraus maps to stabilize any types of states has also been established [35], 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 [55], [49]. 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 [63].

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 [39] for the adiabatic elimination of low-Q cavity). Conversely 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 [46] and invariant manifold techniques [41] 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 [58] will be investigated. They will provide estimates of convergence rates for slightly open quantum systems. We expect that such estimates will help to understand the dependence on the experimental parameters of the convergence rates observed in [52][9] [64].

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.

SPHINX Project-Team

3. Research Program

3.1. Control and stabilization of heterogeneous systems

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

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

In order to control such FSIS systems, one has first to analyze the corresponding system of PDE. The oldest works on FSIS go back to the pioneering contributions of Thomson, Tait and Kirchhoff in the 19th century and Lamb in the 20th century, who considered simplified models (potential fluid or Stokes system). The first mathematical studies in the case of a viscous incompressible fluid modeled by the Navier-Stokes system and a rigid body whose dynamics is modeled by Newton's laws appeared much later [95], [90], [72], and almost all mathematical results on such FSIS have been obtained in the last twenty years.

The most studied FSIS is the problem modeling a **rigid body moving into a viscous incompressible fluid** ([55], [51], [89], [61], [66], [92], [94], [79], [64]). Many other FSIS have been studied as well. Let us mention [81], [69], [65], [54], [44], [60], [45], [62] for different fluids. The case of **deformable structures** has also been considered, either for a fluid inside a moving structure (e.g. blood motion in arteries) or for a moving deformable structure immersed in a fluid (e.g. fish locomotion). The obtained coupled FSIS is a complex system and its study raises several difficulties. The main one comes from the fact that we gather two systems of different nature. Some studies have been performed for approximations of this system: [49], [44], [75], [56], [47]). Without approximations, the only known results [52], [53] is done with very strong assumptions on the regularity of the initial data. Such assumptions are not satisfactory but seem inherent to this coupling between two systems of different natures. In order to study self-propelled motions of structures in a fluid, like fish locomotion, one can assume that the **deformation of the structure is prescribed and known**, whereas its displacement remains unknown ([87]). This permits to start the mathematical study of a challenging problem: understanding the locomotion mechanism of aquatic animals. This is related to control or stabilization problems for FSIS. Some first results in this direction were obtained in [70], [46], [83].

3.2. Inverse problems for heterogeneous systems

The area of inverse problems covers a large class of theoretical and practical issues which are important in many applications (see for instance the books of Isakov [71] or Kaltenbacher, Neubauer, and Scherzer [73]). Roughly speaking, an inverse problem is a problem where one attempts to recover an unknown property of a given system from its response to an external probing signal. For systems described by evolution PDE, one can be interested in the reconstruction from partial measurements of the state (initial, final or current), the inputs (a source term, for instance) or the parameters of the model (a physical coefficient for example). For stationary or periodic problems (i.e. problems where the time dependence is given), one can be interested in determining from boundary data a local heterogeneity (shape of an obstacle, value of a physical coefficient describing the medium, etc.). Such inverse problems are known to be generally ill-posed and their study leads to investigate the following questions:

- *Uniqueness.* The question here is to know whether the measurements uniquely determine the unknown quantity to be recovered. This theoretical issue is a preliminary step in the study of any inverse problem and can be a hard task.
- *Stability.* When uniqueness is ensured, the question of stability, which is closely related to sensitivity, deserves special attention. Stability estimates provide an upper bound for the parameter error given some uncertainty on data. This issue is closely related to the so-called observability inequality in systems theory.
- *Reconstruction.* Inverse problems being usually ill-posed, one needs to develop specific reconstruction algorithms which are robust to noise, disturbances and discretization. A wide class of methods is based on optimization techniques.

We can split our research in inverse problems into two classes which both appear in FSIS and CWS:

1. **Identification for evolution PDE.**

   Driven by applications, the identification problem for systems of infinite dimension described by evolution PDE has seen in the last three decades a fast and significant growth. The unknown to be recovered can be the (initial/final) state (e.g. state estimation problems [39], [63], [67], [91] for the design of feedback controllers), an input (for instance source inverse problems [36], [48], [57]) or a parameter of the system. These problems are generally ill-posed and many regularization approaches have been developed. Among the different methods used for identification, let us mention optimization techniques ([50]), specific one-dimensional techniques (like in [40]) or observer-based methods as in [77].

   In the last few years, we have developed observers to solve initial data inverse problems for a class of linear systems of infinite dimension. Let us recall that observers, or Luenberger observers [76], have been introduced in automatic control theory to estimate the state of a dynamical system of finite dimension from the knowledge of an output (for more references, see for instance [80] or [93]). Using observers, we have proposed in [82], [68] an iterative algorithm to reconstruct initial data from partial measurements for some evolution equations.We are deepening our activities in this direction by considering more general operators or more general sources and the reconstruction of coefficients for the wave equation. In connection with this problem, we study the stability in the determination of these coefficients. To achieve this, we use geometrical optics, which is a classical albeit powerful tool to obtain quantitative stability estimates on some inverse problems with a geometrical background, see for instance [42], [41].

2. **Geometric inverse problems.**

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

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

   where L is a given partial differential operator describing the physical phenomenon under consideration (typically a second order differential operator), B the (possibly unknown) operator describing the boundary condition on the boundary of the heterogeneity and f the exterior source used to probe the medium. The question is then to recover the shape of ω and/or the boundary operator B from some measurement Mu on the outer boundary $\partial\Omega$. This setting includes in particular inverse scattering problems in acoustics and electromagnetics (in this case Ω is the whole space and the data are far

field measurements) and the inverse problem of detecting solids moving in a fluid. It also includes, with slight modifications, more general situations of incomplete data (i.e. measurements on part of the outer boundary) or penetrable inhomogeneities. Our approach to tackle this type of problems is based on the derivation of a series expansion of the input-to-output map of the problem (typically the Dirichlet-to-Neumann map of the problem for the Calderón problem) in terms of the size of the obstacle.

3.3. Numerical analysis and simulation of heterogeneous systems

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

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

Below, we explain in detail the corresponding scientific program.

- **Simulation of FSIS:** In order to simulate fluid-structure systems, one has to deal with the fact that the fluid domain is moving and that the two systems for the fluid and for the structure are strongly coupled. To overcome this free boundary problem, three main families of methods are usually applied to numerically compute in an efficient way the solutions of the fluid-structure interaction systems. The first method consists in suitably displacing the mesh of the fluid domain in order to follow the displacement and the deformation of the structure. A classical method based on this idea is the A.L.E. (Arbitrary Lagrangian Eulerian) method: with such a procedure, it is possible to keep a good precision at the interface between the fluid and the structure. However, such methods are difficult to apply for large displacements (typically the motion of rigid bodies). The second family of methods consists in using a *fixed mesh* for both the fluid and the structure and to simultaneously compute the velocity field of the fluid with the displacement velocity of the structure. The presence of the structure is taken into account through the numerical scheme. Finally, the third class of methods consists in transforming the set of PDEs governing the flow into a system of integral equations set on the boundary of the immersed structure. The members of SPHINX have already worked on these three families of numerical methods for FSIS systems with rigid bodies (see e.g. [86], [74], [88], [84], [85], [78]).
- **Simulation of CWS:** Solving acoustic or electromagnetic scattering problems can become a tremendously hard task in some specific situations. In the high frequency regime (i.e. for small wavelength), acoustic (Helmholtz's equation) or electromagnetic (Maxwell's equations) scattering problems are known to be difficult to solve while being crucial for industrial applications (e.g. in aeronautics and aerospace engineering). Our particularity is to develop new numerical methods based on the hybridization of standard numerical techniques (like algebraic preconditioners, etc.) with approaches borrowed from asymptotic microlocal analysis. Most particularly, we contribute to building hybrid algebraic/analytical preconditioners and quasi-optimal Domain Decomposition Methods (DDM) [43], [58], [59] for highly indefinite linear systems. Corresponding three-dimensional solvers (like for example GetDDM) will be developed and tested on realistic configurations (e.g. submarines, complete or parts of an aircraft, etc.) provided by industrial partners (Thales, Airbus). Another situation where scattering problems can be hard to solve is the one of dense multiple (acoustic, electromagnetic or elastic) scattering media. Computing waves in such media requires us to take into account not only the interactions between the incident wave and the scatterers, but also the effects of the interactions between the scatterers themselves. When the number of scatterers is very large (and possibly at high frequency [38], [37]), specific deterministic or stochastic numerical methods and algorithms are needed. We introduce new optimized numerical methods for solving such complex

configurations. Many applications are related to this problem *e.g.* for osteoporosis diagnosis where quantitative ultrasound is a recent and promising technique to detect a risk of fracture. Therefore, numerical simulation of wave propagation in multiple scattering elastic media in the high frequency regime is a very useful tool for this purpose.

TRIPOP Team

3. Research Program

3.1. Introduction

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

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

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

3.2. Axis 1: Modeling and analysis

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

3.2.1. Multibody vibro-impact systems

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

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

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

3.2.2. Excitable systems

Participants: A. Tonnelier, G. James

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

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

3.2.3. Nonsmooth geomechanics and natural hazards assessment

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

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

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

3.2.4. Cyber-physical systems (hybrid systems)

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

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

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

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

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

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

3.3. Axis 2: Numerical methods and simulation

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

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

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

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

The objective of this research item is to continue to improve classical time–stepping schemes for nonsmooth systems to ensure some qualitative properties in discrete-time. In particular, the following points will be developed

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

3.3.2. Stability and numerical continuation of invariants

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

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

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

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

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

3.3.3. Numerical optimization for discrete nonsmooth problems

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

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

3.4. Axis 3: Automatic Control

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

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

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

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

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

3.4.2. Optimal Control

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

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

3.4.3. Control of nonsmooth discrete Lagrangian systems

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

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

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

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

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

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

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

TROPICAL Project-Team

3. Research Program

3.1. Optimal control and zero-sum games

The dynamic programming approach allows one to analyze one or two-player dynamic decision problems by means of operators, or partial differential equations (Hamilton–Jacobi or Isaacs PDEs), describing the time evolution of the value function, i.e., of the optimal reward of one player, thought of as a function of the initial state and of the horizon. We work especially with problems having long or infinite horizon, modelled by stopping problems, or ergodic problems in which one optimizes a mean payoff per time unit. The determination of optimal strategies reduces to solving nonlinear fixed point equations, which are obtained either directly from discrete models, or after a discretization of a PDE.

The geometry of solutions of optimal control and game problems Basic questions include, especially for stationary or ergodic problems, the understanding of existence and uniqueness conditions for the solutions of dynamic programming equations, for instance in terms of controllability or ergodicity properties, and more generally the understanding of the structure of the full set of solutions of stationary Hamilton–Jacobi PDEs and of the set of optimal strategies. These issues are already challenging in the one-player deterministic case, which is an application of choice of tropical methods, since the Lax-Oleinik semigroup, i.e., the evolution semigroup of the Hamilton-Jacobi PDE, is a linear operator in the tropical sense. Recent progress in the deterministic case has been made by combining dynamical systems and PDE techniques (weak KAM theory [85]), and also using metric geometry ideas (abstract boundaries can be used to represent the sets of solutions [100], [4]). The two player case is challenging, owing to the lack of compactness of the analogue of the Lax-Oleinik semigroup and to a richer geometry. The conditions of solvability of ergodic problems for games (for instance, solvability of ergodic Isaacs PDEs), and the representation of solutions are only understood in special cases, for instance in the finite state space case, through tropical geometry and non-linear Perron-Frobenius methods [47],[14], [3].

Algorithmic aspects: from combinatorial algorithms to the attenuation of the curse of dimensionality Our general goal is to push the limits of solvable models by means of fast algorithms adapted to large scale instances. Such instances arise from discrete problems, in which the state space may so large that it is only accessible through local oracles (for instance, in some web ranking applications, the number of states may be the number of web pages) [86]. They also arise from the discretization of PDEs, in which the number of states grows exponentially with the number of degrees of freedom, according to the "curse of dimensionality". A first line of research is the development of *new approximation methods for the value function*. So far, classical approximations by linear combinations have been used, as well as approximation by suprema of linear or quadratic forms, which have been introduced in the setting of dual dynamic programming and of the so called "max-plus basis methods" [87]. We believe that more concise or more accurate approximations may be obtained by unifying these methods. Also, some max-plus basis methods have been shown to *attenuate the curse of dimensionality* for very special problems (for instance involving switching) [108], [92]. This suggests that the complexity of control or games problems may be measured by more subtle quantities that the mere number of states, for instance, by some forms of metric entropy (for example, certain large scale problems have a low complexity owing to the presence of decomposition properties, "highway hierarchies", etc.). A second line of of our research is the development of *combinatorial algorithms*, to solve large scale zero-sum two-player problems with discrete state space. This is related to current open problems in algorithmic game theory. In particular, the existence of polynomial-time algorithms for games with ergodic payment is an open question. See e.g. [53] for a polynomial time average complexity result derived by tropical methods. The two lines of research are related, as the understanding of the geometry of solutions allows to develop better approximation or combinatorial algorithms.

3.2. Non-linear Perron-Frobenius theory, nonexpansive mappings and metric geometry

Several applications (including population dynamics [9] and discrete event systems [62], [70], [55]) lead to studying classes of dynamical systems with remarkable properties: preserving a cone, preserving an order, or being nonexpansive in a metric. These can be studied by techniques of non-linear Perron-Frobenius theory [3] or metric geometry [10]. Basic issues concern the existence and computation of the "escape rate" (which determines the throughput, the growth rate of the population), the characterizations of stationary regimes (non-linear fixed points), or the study of the dynamical properties (convergence to periodic orbits). Nonexpansive mappings also play a key role in the "operator approach" to zero-sum games, since the one-day operators of games are nonexpansive in several metrics, see [8].

3.3. Tropical algebra and convex geometry

The different applications mentioned in the other sections lead us to develop some basic research on tropical algebraic structures and in convex and discrete geometry, looking at objects or problems with a "piecewise-linear " structure. These include the geometry and algorithmics of tropical convex sets [58], [50], tropical semialgebraic sets [60], the study of semi-modules (analogues of vector spaces when the base field is replaced by a semi-field), the study of systems of equations linear in the tropical sense, investigating for instance the analogues of the notions of rank, the analogue of the eigenproblems [52], and more generally of systems of tropical polynomial equations. Our research also builds on, and concern, classical convex and discrete geometry methods.

3.4. Tropical methods applied to optimization, perturbation theory and matrix analysis

Tropical algebraic objects appear as a deformation of classical objects thought various asymptotic procedures. A familiar example is the rule of asymptotic calculus,

$$e^{-a/\epsilon} + e^{-b/\epsilon} \asymp e^{-\min(a,b)/\epsilon} \ , \qquad e^{-a/\epsilon} \times e^{-b/\epsilon} = e^{-(a+b)/\epsilon} \ , \tag{43}$$

when $\epsilon \to 0^+$. Deformations of this kind have been studied in different contexts: large deviations, zero-temperature limits, Maslov's "dequantization method" [107], non-archimedean valuations, log-limit sets and Viro's patchworking method [132], etc.

This entails a relation between classical algorithmic problems and tropical algorithmic problems, one may first solve the $\epsilon = 0$ case (non-archimedean problem), which is sometimes easier, and then use the information gotten in this way to solve the $\epsilon = 1$ (archimedean) case.

In particular, tropicalization establishes a connection between polynomial systems and piecewise affine systems that are somehow similar to the ones arising in game problems. It allows one to transfer results from the world of combinatorics to "classical" equations solving. We investigate the consequences of this correspondence on complexity and numerical issues. For instance, combinatorial problems can be solved in a robust way. Hence, situations in which the tropicalization is faithful lead to improved algorithms for classical problems. In particular, scalings for the polynomial eigenproblems based on tropical preprocessings have started to be used in matrix analysis [93], [98].

Moreover, the tropical approach has been recently applied to construct examples of linear programs in which the central path has an unexpectedly high total curvature [54], and it has also led to positive polynomial-time average case results concerning the complexity of mean payoff games. Similarly, we are studying semidefinite programming over non-archimedean fields [60], [59], with the goal to better understand complexity issues in classical semidefinite and semi-algebraic programming.

BONUS Team

3. Research Program

3.1. Decomposition-based Optimization

Given the large scale of the targeted optimization problems in terms of the number of variables and objectives, their decomposition into simplified and loosely coupled or independent subproblems is essential to raise the challenge of scalability. The first line of research is to *investigate the decomposition approach in the two spaces and their combination, as well as their implementation on ultra-scale architectures*. The motivation of the decomposition is twofold: first, the decomposition allows the parallel resolution of the resulting subproblems on ultra-scale architectures. Here also several issues will be addressed: the definition of the subproblems, their coding to allow their efficient communication and storage (checkpointing), their assignment to processing cores, etc. Second, decomposition is necessary for solving large problems that cannot be solved (efficiently) using traditional algorithms. Indeed, for instance with the popular NSGA-II algorithm the number of non-dominated solutions [0] increases drastically with the number of objectives leading to a very slow convergence to the Pareto front [0]. Therefore, decomposition-based techniques are gaining a growing interest. The objective of BONUS is to *investigate various decomposition schema and cooperation protocols between the subproblems* resulting from the decomposition to generate efficiently global solutions of good quality. Several challenges have to be addressed: how to define the subproblems (decomposition strategy), how to solve them to generate local solutions (local rules), and how to combine these latter with those generated by other subproblems and how to generate global solutions (cooperation mechanism), and how to combine decomposition strategies in more than one space (hybridization strategy)? These challenges, which are in the line with the CIS Task Force [0] on decomposition will be addressed in the decision as well as in the objective space.

The *decomposition in the decision space* can be performed following different ways according to the problem at hand. Two major categories of decomposition techniques can be distinguished: the first one consists in *breaking down the high-dimensional decision vector* into low-dimensional and easier-to-optimize blocks of variables. The major issue is how to define the subproblems (blocks of variables) and their cooperation protocol: randomly *vs.* using some learning (e.g. separability analysis), statically *vs.* adaptively, etc. *The decomposition in the decision space can also be guided by the type of variables i.e. discrete vs. continuous*. The discrete and continuous parts are optimized separately using cooperative hybrid algorithms [47]. *The major issue of this kind of decomposition is the presence of categorial variables in the discrete part [33]. The* BONUS *team is addressing this issue, rarely investigated in the literature*, within the context of vehicle aerospace engineering design. The second category consists in the *decomposition according to the ranges of the decision variables*. For continuous problems, the idea consists in iteratively subdividing the search (e.g. design) space into subspaces (hyper-rectangles, intervals, etc.) and select those that are most likely to produce the lowest objective function value. *Existing approaches meet increasing difficulty with an increasing number of variables and are often applied to low-dimensional problems. We are investigating this scalability challenge* (e.g. [10]). *For discrete problems, the major challenge is to find a coding (mapping) of the search space to a decomposable entity*. We have proposed an interval-based coding of the permutation space for solving big permutation problems. The approach opens perspectives we are investigating [7], in terms of ultra-scale parallelization, application to multi-permutation problems and hybridization with metaheuristics.

[0] A solution x dominates another solution y if x is better than y for all objectives and there exists at least one objective for which x is strictly better than y.
[0] A Pareto Front is the set of non-dominated solutions.
[0] IEEE CIS Task Force, created in 2017 on Decomposition-based Techniques in Evolutionary Computation.

The *decomposition in the objective space* consists in breaking down an original MaOP into a set of cooperative single-objective subproblems (SOPs). The decomposition strategy requires the careful definition of a scalarizing (aggregation) function and its weighting vectors (each of them corresponds to a separate SOP) to guide the search process towards the best regions. Several scalarizing functions have been proposed in the literature including weighted sum, weighted Tchebycheff, vector angle distance scaling, etc. These functions are widely used but they have their limitations. For instance, using weighted Tchebycheff might do harm diversity maintenance and weighted sum is inefficient when it comes to deal with nonconvex Pareto Fronts [40]. Defining a scalarizing function well-suited to the MaOP at hand is therefore a difficult and still an open question being investigated in BONUS [6], [5]. Studying/defining various functions and in-depth analyzing them to better understand the differences between them is required. Regarding the weighting vectors that determine the search direction, their efficient setting is also a key and open issue. They dramatically affect in particular the diversity performance. Their setting rises several issues mainly: how to determine their number according to the available computational ressources? when (statically or adaptively) and how to determine their values? *Weight adaptation is one of our main concerns that we are addressing especially from a distributed perspective.* They correspond to the main scientific objectives targeted by our bilateral ANR-RGC BigMO project with City University (Hong Kong). The other challenges pointed out in the beginning of this section concern the way to solve locally the SOPs resulting from the decomposition of a MaOP and the mechanism used for their cooperation to generate global solutions. To deal with these challenges, our approach is to design the decomposition strategy and cooperation mechanism keeping in mind the parallel and/or distributed solving of the SOPs. Indeed, we favor the local neighborhood-based mating selection and replacement to minimize the network communication cost while allowing an effective resolution [5]. The major issues here are how to define the neighborhood of a subproblem and how to cooperatively update the best-known solution of each subproblem and its neighbors.

To sum up, the objective of the BONUS *team is to come up with scalable decomposition-based approaches in the decision and objective spaces. In the decision space, a particular focus will be put on high dimensionality and mixed-continuous variables which have received little interest in the literature. We will particularly continue to investigate at larger scales using ultra-scale computing the interval-based (discrete) and fractal-based (continuous) approaches. We will also deal with the rarely addressed challenge of mixed-continuous including categorial variables (collaboration with ONERA). In the objective space, we will investigate parallel ultra-scale decomposition-based many-objective optimization with ML-based adaptive building of scalarizing functions. A particular focus will be put on the state-of-the-art MOEA/D algorithm. This challenge is rarely addressed in the literature which motivated the collaboration with the designer of MOEA/D (bilateral ANR-RGC BigMO project with City University, Hong Kong). Finally, the joint decision-objective decomposition, which is still in its infancy [49], is another challenge of major interest.*

3.2. Machine Learning-assisted Optimization

The Machine Learning (ML) approach based on metamodels (or surrogates) is commonly used, and also adopted in BONUS, to assist optimization in tackling BOPs characterized by time-demanding objective functions. The second line of research of BONUS is focused on ML-aided optimization to raise the challenge of expensive functions of BOPs using surrogates but also to assist the two other research lines (decomposition-based and ultra-scale optimization) in dealing with the other challenges (high dimensionality and scalability).

Several issues have been identified to make efficient and effective surrogate-assisted optimization. First, infill criteria have to be carefully defined to adaptively select the adequate sample points (in terms of surrogate precision and solution quality). The challenge is to find the best trade-off between exploration and exploitation to efficiently refine the surrogate and guide the optimization process toward the best solutions. The most popular infill criterion is probably the *Expected Improvement* (EI) [43] which is based on the expected values of sample points but also and importantly on their variance. This latter is inherently determined in the kriging model, this is why it is used in the state-of-the-art *efficient global optimization* (EGO) algorithm [43]. However, such crucial information is not provided in all surrogate models (e.g. ANN) and needs to be derived. In BONUS, we are currently investigating this issue. Second, it is known that surrogates allow one to reduce the

computational burden for solving BOPs with time-demanding function(s). However, using parallel computing as a complementary way is often recommended and cited as a perspective in the conclusions of related publications. Nevertheless, *despite being of critical importance parallel surrogate-assisted optimization is weakly addressed in the literature*. For instance, in the introduction of the survey proposed in [42] it is warned that because the area is not mature yet the paper is more focused on the potential of the surveyed approaches than on their relative efficiency. *Parallel computing is required at different levels that we are investigating*.

Another issue with surrogate-assisted optimization is related to high dimensionality in decision as well as in objective space: it is often applied to low-dimensional problems. *The joint use of decomposition, surrogates and massive parallelism is an efficient approach to deal with high dimensionality. This approach adopted in* BONUS *has received little effort in the literature.* In BONUS, we are considering a generic framework in order to enable a flexible coupling of existing surrogate models within the state-of-the-art decomposition-based algorithm MOEA/D. This is a first step in leveraging the applicability of efficient global optimization into the multi-objective setting through parallel decomposition. Another issue which is a consequence of high dimensionality is the mixed (discrete-continuous) nature of decision variables which is frequent in real-world applications (e.g. engineering design). *While surrogate-assisted optimization is widely applied in the continuous setting it is rarely addressed in the literature in the discrete-continuous framework.* In [33], we have identified different ways to deal with this issue that we are investigating. Non-stationary functions frequent in real-world applications (see Section 4.1) is another major issue we are addressing using the concept of deep GP.

Finally, as quoted in the beginning of this section, ML-assisted optimization is mainly used to deal with BOPs with expensive functions but it will also be investigated for other optimization tasks. Indeed, ML will be useful to assist the decomposition process. In the decision space, it will help to perform the separability analysis (understanding of the interactions between variables) to decompose the vector of variables. In the objective space, ML will be useful to assist a decomposition-based many-objective algorithm in dynamically selecting a scalarizing function or updating the weighting vectors according to their performances in the previous steps of the optimization process [5]. Such a data-driven ML methodology would allow us to understand what makes a problem difficult or an optimization approach efficient, to predict the algorithm performance [4], to select the most appropriate algorithm configuration [8], and to adapt and improve the algorithm design for unknown optimization domains and instances. Such an autonomous optimization approach would adaptively adjust its internal mechanisms in order to tackle cross-domain BOPs.

In a nutshell, to deal with expensive optimization the BONUS *team will investigate the surrogate-based ML approach with the objective to efficiently integrate surrogates in the optimization process. The focus will especially be put on high dimensionality (e.g. using decomposition) with mixed discrete-continuous variables which is rarely investigated. The kriging metamodel (Gaussian Process or GP) will be considered in particular for engineering design (for more reliability) addressing the above issues and other major ones including mainly non stationarity (using emerging deep GP) and ultra-scale parallelization (highly needed by the community). Indeed, a lot of work has been reported on deep neural networks (deep learning) surrogates but not on the others including (Deep) GP. On the other hand, ML will be used to assist decomposition: importance/interaction between variables in the decision space, dynamic building (selection of scalarizing functions, weight update, ...) of scalarizing functions in the objective space, etc.*

3.3. Ultra-scale Optimization

The third line of our research program that accentuates our difference from other (project-)teams of the related Inria scientific theme is the ultra-scale optimization. *This research line is complementary to the two others, which are sources of massive parallelism* and with which it should be combined to solve BOPs. Indeed, ultra-scale computing is necessary for the effective resolution of the large amount of subproblems generated by decomposition of BOPs, parallel evaluation of simulation-based fitness and metamodels, etc. These sources of parallelism are attractive for solving BOPs and are natural candidates for ultra-scale supercomputers [0].

However, their efficient use raises a big challenge consisting in managing efficiently a massive amount of irregular tasks on supercomputers with multiple levels of parallelism and heterogeneous computing resources (GPU, multi-core CPU with various architectures) and networks. Raising such challenge requires to tackle three major issues, scalability, heterogeneity and fault-tolerance, discussed in the following.

The *scalability* issue requires, on the one hand, the definition of scalable data structures for efficient storage and management of the tremendous amount of subproblems generated by decomposition [45]. On the other hand, achieving extreme scalability requires also the optimization of communications (in number of messages, their size and scope) especially at the inter-node level. For that, we target the design of asynchronous locality-aware algorithms as we did in [41], [48]. In addition, efficient mechanisms are needed for granularity management and coding of the work units stored and communicated during the resolution process.

Heterogeneity means harnessing various resources including multi-core processors within different architectures and GPU devices. The challenge is therefore to design and implement hybrid optimization algorithms taking into account the difference in computational power between the various resources as well as the resource-specific issues. On the one hand, to deal with the heterogeneity in terms of computational power, we adopt in BONUS the dynamic load balancing approach based on the Work Stealing (WS) asynchronous paradigm [0] at the inter-node as well as at the intra-node level. We have already investigated such approach, with various victim selection and work sharing strategies in [48], [7]. On the other hand, hardware resource specific-level optimization mechanisms are required to deal with related issues such as thread divergence and memory optimization on GPU, data sharing and synchronization, cache locality, and vectorization on multi-core processors, etc. These issues have been considered separately in the literature including our works [9], [1]. Indeed, in most of existing works related to GPU-accelerated optimization only a single CPU core is used. This leads to a huge resource wasting especially with the increase of the number of processing cores integrated into modern processors. Using jointly the two components raises additional issues including data and work partitioning, the optimization of CPU-GPU data transfers, etc.

Another issue the scalability induces is the *increasing probability of failures* in modern supercomputers [46]. Indeed, with the increase of their size to millions of processing cores their MTBF tends to be shorter and shorter [44]. Failures may have different sources including hardware and software faults, silent errors, etc. In our context, we consider failures leading to the loss of work unit(s) being processed by some thread(s) during the resolution process. The major issue, which is particularly critical in exact optimization, is how to recover the failed work units to ensure a reliable execution. Such issue is tackled in the literature using different approaches: algorithm-based fault tolerance, checkpoint/restart (CR), message logging and redundancy. The CR approach can be system-level, library/user-level or application-level. Thanks to its efficiency in terms of memory footprint, adopted in BONUS [2], the application-level approach is commonly and widely used in the literature. This approach raises several issues mainly: what is critical information which defines the state of the work units and allows to resume properly their execution? when, where and how (using which data structures) to store it efficiently? how to deal with the two other issues: scalability and heterogeneity?

The last but not least major issue which is another roadblock to exascale is the programming of massive-scale applications for modern supercomputers. *On the path to exascale, we will investigate the programming environments and execution supports able to deal with exascale challenges: large numbers of threads, heterogeneous resources, etc.* Various exascale programming approaches are being investigated by the parallel computing community and HPC builders: extending existing programming languages (e.g. DSL-C++) and environments/libraries (MPI+X, etc.), proposing new solutions including mainly PGAS-based environments (Chapel, UPC, X10, etc.). It is worth noting here that our objective is not to develop a programming environment nor a runtime support for exascale computing. Instead, we aim to collaborate with the research teams (inside or outside Inria) having such objective.

[0] In the context of BONUS, supercomputers are composed of several massively parallel processing nodes (inter-node parallelism) including multi-core processors and GPUs (intra-node parallelism).

[0] A WS mechanism is mainly defined by two components: a victim selection strategy which selects the processing core to be stolen and a work sharing policy which determines the part and amount of the work unit to be given to the thief upon WS request.

To sum up, we put the focus on the design and implementation of efficient big optimization algorithms dealing jointly (uncommon in parallel optimization) with the major issues of ultra-scale computing mainly the scalability up to millions of cores using scalable data structures and asynchronous locality-aware work stealing, heterogeneity addressing the multi-core and GPU-specific issues and those related to their combination, and scalable GPU-aware fault tolerance. A strong effort will be devoted to this latter challenge, for the first time to the best of our knowledge, using application-level checkpoint/restart approach to deal with failures.

GEOSTAT Project-Team

3. Research Program

3.1. General methodology

Fully Developed Turbulence (FDT) Turbulence at very high Reynolds numbers; systems in FDT are beyond deterministic chaos, and symmetries are restored in a statistical sense only, and multi-scale correlated structures are landmarks. Generalizing to more random uncorrelated multi-scale structured turbulent fields.

Compact Representation Reduced representation of a complex signal (dimensionality reduction) from which the whole signal can be reconstructed. The reduced representation can correspond to points randomly chosen, such as in Compressive Sensing, or to geometric localization related to statistical information content (framework of reconstructible systems).

Sparse representation The representation of a signal as a linear combination of elements taken in a dictionary (frame or Hilbertian basis), with the aim of finding as less as possible non-zero coefficients for a large class of signals.

Universality class In theoretical physics, the observation of the coincidence of the critical exponents (behaviour near a second order phase transition) in different phenomena and systems is called universality. Universality is explained by the theory of the renormalization group, allowing for the determination of the changes followed by structured fluctuations under rescaling, a physical system is the stage of. The notion is applicable with caution and some differences to generalized out-of-equilibrium or disordered systems. Non-universal exponents (without definite classes) exist in some universal slowing dynamical phenomena like the glass transition and kindred. As a consequence, different macroscopic phenomena displaying multiscale structures (and their acquisition in the form of complex signals) may be grouped into different sets of generalized classes.

Every signal conveys, as a measure experiment, information on the physical system whose signal is an acquisition of. As a consequence, it seems natural that signal analysis or compression should make use of physical modelling of phenomena: the goal is to find new methodologies in signal processing that goes beyond the simple problem of interpretation. Physics of disordered systems, and specifically physics of (spin) glasses is putting forward new algorithmic resolution methods in various domains such as optimization, compressive sensing etc. with significant success notably for NP hard problem heuristics. Similarly, physics of turbulence introduces phenomenological approaches involving multifractality. Energy cascades are indeed closely related to geometrical manifolds defined through random processes. At these structures' scales, information in the process is lost by dissipation (close to the lower bound of inertial range). However, all the cascade is encoded in the geometric manifolds, through long or short distance correlations depending on cases. How do these geometrical manifold structures organize in space and time, in other words, how does the scale entropy cascades itself ? To unify these two notions, a description in term of free energy of a generic physical model is sometimes possible, such as an elastic interface model in a random nonlinear energy landscape : This is for instance the correspondence between compressible stochastic Burgers equation and directed polymers in a disordered medium. Thus, trying to unlock the fingerprints of cascade-like structures in acquired natural signals becomes a fundamental problem, from both theoretical and applicative viewpoints.

To illustrate the general methodology undertaken, let us focus on an example conducted in the study of physiological time series: the analysis of signals recorded from the electrical activity of the heart in the general setting of Atrial Fibrillation (AF). AF is a cardiac arrhythmia characterized by rapid and irregular atrial electrical activity with a high clinical impact on stroke incidence. Best available therapeutic strategies combine pharmacological and surgical means. But when successful, they do not always prevent long-term relapses.

Initial success becomes all the more tricky to achieve as the arrhythmia maintains itself and the pathology evolves into sustained or chronic AF. This raises the open crucial issue of deciphering the mechanisms that govern the onset of AF as well as its perpetuation. We have developed a wavelet-based multi-scale strategy to analyze the electrical activity of human hearts recorded by catheter electrodes, positioned in the coronary sinus (CS), during episodes of chronic AF. We have computed the so-called multifractal spectra using two variants of the wavelet transform modulus maxima method, the moment (partition function) method and the magnitude cumulant method (checking confidence intervals with surrogate data). Application of these methods to long time series recorded in a patient with chronic AF provides quantitative evidence of the multifractal intermittent nature of the electric energy of passing cardiac impulses at low frequencies, *i.e.* for times ($>\sim 0.5$ s) longer than the mean interbeat ($\simeq 10^{-1}$s). We have also reported the results of a two-point magnitude correlation analysis which infers the absence of a multiplicative time-scale structure underlying multifractal scaling. The electric energy dynamics looks like a "multifractal white noise" with quadratic (log-normal) multifractal spectra. *These observations challenge concepts of functional reentrant circuits in mechanistic theories of AF*. A transition is observed in the computed multifractal spectra which group according to two distinct areas, consistently with the anatomical substrate binding to the CS, namely the left atrial posterior wall, and the ligament of Marshall which is innervated by the ANS. These negative results challenge also the existing models, which by principle cannot explain such results. As a consequence, we go beyond the existing models and propose a mathematical model of a denervated heart where the kinetics of gap junction conductance alone induces a desynchronization of the myocardial excitable cells, accounting for the multifractal spectra found experimentally in the left atrial posterior wall area (devoid of ANS influence).

3.2. Multiscale description in terms of multiplicative cascade, application to Earth observation signals

The research described in this section is a collaboration effort of GEOSTAT, CNRS LEGOS (Toulouse), CNRS LAM (Marseille Laboratory for Astrophysics), MERCATOR (Toulouse), IIT Roorkee, Moroccan Royal Center for Teledetection (CRST), Moroccan Center for Science CNRST, Rabat University, University of Heidelberg. Researchers involved:

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The analysis and modeling of natural phenomena, specially those relevant to geophysical sciences, are influenced by statistical and multiscale phenomenological descriptions of turbulence; indeed these descriptions are able to explain the partition of energy within a certain range of scales. A particularly important aspect of the statistical theory of turbulence lies in the discovery that the support of the energy transfer is spatially highly non uniform, in other terms it is *intermittent* [67]. 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 [64] 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 [34], [60]. Some quantities related to nonlinearity, such as Lyapunov exponents, Kolmogorov-Sinai entropy etc. can be computed at least in the phase space [35]. 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 Takens-81 about strange attractors in transition turbulence has motivated 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. 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 [13] and to deduce relevant information associated to multiscale geophysical signals [14]. A multiscale organization is a fundamental feature of a complex system, it can be for example related to the cascading properties in turbulent systems. We make use of this kind of description when analyzing turbulent signals: intermittency is observed within the inertial range and is related to the fact that, in the case of FDT (fully developed turbulence), symmetry is restored only in a statistical sense, a fact that has consequences on the quality of any nonlinear signal representation by frames or dictionaries.

The example of FDT as a standard "template" for developing general methods that apply to a vast class of complex systems and signals is of fundamental interest because, in FDT, the existence of a multiscale hierarchy $\mathcal{F}_h$ which is of multifractal nature and geometrically localized can be derived from physical considerations. This geometric hierarchy of sets is responsible for the shape of the computed singularity spectra, which in turn is related to the statistical organization of information content in a signal. It explains scale invariance, a characteristic feature of complex signals. The analogy from statistical physics comes from the fact that singularity exponents are direct generalizations of *critical exponents* which explain the macroscopic properties of a system around critical points, and the quantitative characterization of *universality classes*, which allow the definition of methods and algorithms that apply to general complex signals and systems, and not only turbulent signals: signals which belong to a same universality class share common statistical organization. During the past decades, canonical approaches 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 [30]. The research goal is to be able to determine universality classes associated to acquired signals, independently of microscopic properties in the phase space of various complex systems, and beyond the particular case of turbulent data [54].

3.3. Excitable systems: analysis of physiological time series

The research described in this section is a collaboration effort of GEOSTAT, CNRS LOMA (Laboratoire Ondes et Matière d'Aquitaine) and Laboratory of Physical Foundation of Strength, Institute of Continuous Media Mechanics (Perm, Russia Federation).

AF is an arrhythmia originating in the rapid and irregular electrical activity of the atria (the heart's two upper chambers) that causes their pump function to fail, increasing up to fivefold the risk of embolic stroke. The prevailing electrophysiological concepts describing tachy-arrhythmias are more than a century old. They involve abnormal automaticity and conduction [53]. Initiation and maintenance are thought to arise from a vulnerable substrate prone to the emergence of multiple self-perpetuating reentry circuits, also called "multiple wavelets" [58], [59]. Reentries may be driven structurally, for instance because of locally high fibrous tissue content which badly conducts, or functionally because of high spatial dispersion of decreased refractoriness and APD [57]. The latter is coined the leading circle concept with the clinically more relevant notion of a

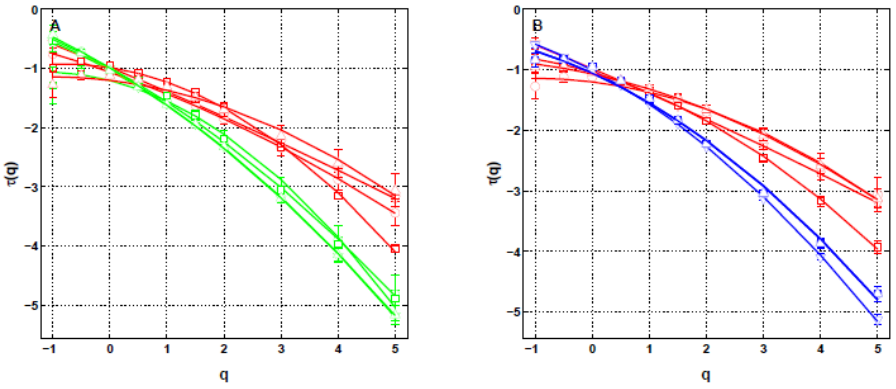

Figure 1. $\tau(q)$ spectra of local impulse energy time-series recorded along the CS vein at the electrodes Pt2 (red), Pt3 (blue) and Pt5 (green). The curves represent quadratic polynomial fit of the data. (A) The symbols correspond to the reference Patient 1 (chronic AF,$\bigtriangledown$), and to Patients 2 (chronic AF, $\circ$) 3 (paroxysmal AF, $\square$) and 4 (persistent AF, $\bigtriangleup$). (B) The symbols correspond to the reference Patient 1 ($\bigtriangledown$) and to three different time-series for Patient 4 ($\circ$,$\square$,$\bigtriangleup$) recorded at different periods of time preceding ablation procedure.

critical "wavelength" (in fact the length) of the cardiac impulse [29], [63], [61], [33]. The related concept of vulnerability was originally introduced to uncover a physiological substrate evolving from normality to pathology. It was found in vulnerable patients that high rate frequency would invariably lead to functional disorder as cardiac cells would no longer properly adapt their refractoriness [32]. Mathematical models have managed to exhibit likewise phenomena, with the generation of breaking spiral waves in various conditions [50], [55]. The triggering role of abnormal ectopic activity of the pulmonary veins has been demonstrated on patients with paroxysmal AF resistant to drug therapy [49], but its origin still remains poorly understood. This region is highly innervated with sympathetic and parasympathetic stimulation from the ANS [65], [66], [31]. In particular, Coumel et al. [41], [40] have revealed the pathophysiological role of the vagal tone on a vulnerable substrate. It is frequently observed that rapid tachycardia of ectopic origin transits to AF. This is known to result from electrical remodeling. As described for the first time by Allessie et al. [28], remodeling is a transient and reversible process by which the impulse properties such as its refractory period are altered during the course of the arrhythmia, promoting its perpetuation: "AF begets AF" [68]. Under substantial beating rate increase, cells may undergo remodeling to overcome the toxicity of their excessive intercellular calcium loading, by a rapid down regulation (a few minutes) of their L-type calcium membrane current. Moreover, other ionic channel functions are also modified such as the potassium channel function, inducing a change in the conduction properties including the conduction velocity. The intercellular coupling at the gap junction level shows also alterations of their connexin expression and dispersion.

Wavelet-based methods (WTMM, log-cumulants, two point scale correlations), and confidence statistical methodology, have been applied to catheter recordings in the coronary sinus vein right next to the left atria of a small sample of patients with various conditions, and exhibit clear multifractal scaling without cross-scale correlation, which are coined "multifractal white noise", and that can be grouped according to two anatomical regions. One of our main result was to show that this is incompatible with the common lore for atrial fibrillation based on so-called circuit reentries. We used two declinations of a wavelet-based multi-scale method, the moment (partition function) method and the magnitude cumulant method, as originally introduced in the field of fully developed turbulence. In the context of cardiac physiology, this methodology was shown to be valuable in assessing congestive heart failure from the monitoring of sinus heart rate variability [51]. We develop a model such that the substrate function is modulated by the kinetics of conduction. A simple reversible

mechanism of short term remodeling under rapid pacing is demonstrated, by which ionic overload acts locally (dynamical feedback) on the kinetics of gap junction conductance. The whole process may propagate and pervade the myocardium via electronic currents, becoming desynchronized. In a new description, we propose that circuit reentries may well exist before the onset of fibrillation, favoring onset but not contributing directly to the onset and perpetuation. By contrast, cell-to-cell coupling is considered fundamentally dynamical. The rationale stems from the observation that multifractal scaling necessitates a high number of degrees of freedom (tending to infinity with system size), which can originate in excitable systems in hyperbolic spatial coupling. See figure 1 .

3.4. Data-based identification of characteristic scales and automated modeling

Data are often acquired at the highest possible resolution, but that scale is not necessarily the best for modeling and understanding the system from which data was measured. The intrinsic properties of natural processes do not depend on the arbitrary scale at which data is acquired; yet, usual analysis techniques operate at the acquisition resolution. When several processes interact at different scales, the identification of their characteristic scales from empirical data becomes a necessary condition for properly modeling the system. A classical method for identifying characteristic scales is to look at the work done by the physical processes, the energy they dissipate over time. The assumption is that this work matches the most important action of each process on the studied natural system, which is usually a reasonable assumption. In the framework of time-frequency analysis [46], the power of the signal can be easily computed in each frequency band, itself matching a temporal scale.

However, in open and dissipative systems, energy dissipation is a prerequisite and thus not necessarily the most useful metric to investigate. In fact, most natural, physical and industrial systems we deal with fall in this category, while balanced quasi-static assumptions are practical approximation only for scales well below the characteristic scale of the involved processes. Open and dissipative systems are not locally constrained by the inevitable rise in entropy, thus allowing the maintaining through time of mesoscopic ordered structures. And, according to information theory [48], more order and less entropy means that these structures have a higher information content than the rest of the system, which usually gives them a high functional role.

We propose to identify characteristic scales not only with energy dissipation, as usual in signal processing analysis, but most importantly with information content. Information theory can be extended to look at which scales are most informative (e.g. multi-scale entropy [39], ε-entropy [38]). Complexity measures quantify the presence of structures in the signal (e.g. statistical complexity [43], MPR [56] and others [45]). With these notions, it is already possible to discriminate between random fluctuations and hidden order, such as in chaotic systems [42], [56]. The theory of how information and structures can be defined through scales is not complete yet, but the state of art is promising [44]. Current research in the team focuses on how informative scales can be found using collections of random paths, assumed to capture local structures as they reach out [37].

Building on these notions, it should also possible to fully automate the modeling of a natural system. Once characteristic scales are found, causal relationships can be established empirically. They are then clustered together in internal states of a special kind of Markov models called ϵ-machines [43]. These are known to be the optimal predictors of a system, with the drawback that it is currently quite complicated to build them properly, except for small system [62]. Recent extensions with advanced clustering techniques [36], [47], coupled with the physics of the studied system (e.g. fluid dynamics), have proved that ϵ-machines are applicable to large systems, such as global wind patterns in the atmosphere [52]. Current research in the team focuses on the use of reproducing kernels, coupled possibly with sparse operators, in order to design better algorithms for ϵ-machines reconstruction. In order to help with this long-term project, a collaboration with J. Crutchfield lab at UC Davis was initiated in 2017.

3.5. Speech analysis

Phonetic and sub-ponethic analysis: We developed a novel algorithm for automatic detection of Glottal Closure Instants (GCI) from speech signals using the Microcanonical Multiscale Formalism (MMF). This state of the

art algorithm is considered as a reference in this field. We made a Matlab code implementing it available to the community (link). Our approach is based on the Microcanonical Multiscale Formalism. We showed that in the case of clean speech, our algorithm performs almost as well as a recent state-of-the-art method. In presence of different types of noises, we showed that our method is considerably more accurate (particularly for very low SNRs). Moreover, our method has lower computational times does not rely on an estimate of pitch period nor any critical choice of parameters. Using the same MMF, we also developed a method for phonetic segmentation of speech signal. We showed that this method outperforms state of the art ones in term of accuracy and efficiency.

Pathological speech analysis and classification: we made a critical analysis of some widely used methodologies in pathological speech classification. We then introduced some novel methods for extracting some common features used in pathological speech analysis and proposed more robust techniques for classification.

Speech analysis of patients with Parkinsonism: with our collaborators from the Czech Republic, we started preliminary studies of some machine learning issues in the field essentially due the small amount of training data.

INOCS Project-Team

3. Research Program

3.1. Introduction

An optimization problem consists in finding a best solution from a set of feasible solutions. Such a problem can be typically modeled as a mathematical program in which decision variables must:

1. satisfy a set of constraints that translate the feasibility of the solution and
2. optimize some (or several) objective function(s). Optimization problems are usually classified according to types of decision to be taken into strategic, tactical and operational problems.

We consider that an optimization problem presents a complex structure when it involves decisions of different types/nature (i.e. strategic, tactical or operational), and/or presenting some hierarchical leader-follower structure. The set of constraints may usually be partitioned into global constraints linking variables associated with the different types/nature of decision and constraints involving each type of variables separately. Optimization problems with a complex structure lead to extremely challenging problems since a global optimum with respect to the whole sets of decision variables and of constraints must be determined.

Significant progresses have been made in optimization to solve academic problems. Nowadays large-scale instances of some NP-Hard problems are routinely solved to optimality. *Our vision within INOCS is to make the same advances while addressing CS optimization problems*. To achieve this goal we aim to develop global solution approaches at the opposite of the current trend. INOCS team members have already proposed some successful methods following this research lines to model and solve CS problems (e.g. ANR project RESPET, Brotcorne *et al.* 2011, 2012, Gendron *et al.* 2009, Strack *et al.* 2009). However, these are preliminary attempts and a number of challenges regarding modeling and methodological issues have still to be met.

3.2. Modeling problems with complex structures

A classical optimization problem can be formulated as follows:

$$\begin{array}{ll} \min & f(x) \\ s.t. & x \in X. \end{array} \tag{44}$$

In this problem, X is the set of feasible solutions. Typically, in mathematical programming, X is defined by a set of constraints. x may be also limited to non-negative integer values.

INOCS team plan to address optimization problem where two types of decision are addressed jointly and are interrelated. More precisely, let us assume that variables x and y are associated with these decisions. A generic model for CS problems is the following:

$$\begin{array}{ll} \min & g(x,y) \\ s.t. & x \in X, \\ (x,y) & \in XY, \\ y & \in Y(x). \end{array} \tag{45}$$

In this model, X is the set of feasible values for x. XY is the set of feasible values for x and y jointly. This set is typically modeled through linking constraints. Last, $Y(x)$ is the set of feasible values for y for a given x. In INOCS, we do not assume that $Y(x)$ has any properties.

The INOCS team plans to model optimization CS problems according to three types of optimization paradigms: large scale complex structures optimization, bilevel optimization and robust/stochastic optimization. These paradigms instantiate specific variants of the generic model.

Large scale complex structures optimization problems can be formulated through the simplest variant of the generic model given above. In this case, it is assumed that $Y(x)$ does not depend on x. In such models, X and Y are associated with constraints on x and on y, XY are the linking constraints. x and y can take continuous or integer values. Note that all the problem data are deterministically known.

Bilevel programs allow the modeling of situations in which a decision-maker, hereafter the leader, optimizes his objective by taking explicitly into account the response of another decision maker or set of decision makers (the follower) to his/her decisions. Bilevel programs are closely related to Stackelberg (leader-follower) games as well as to the principal-agent paradigm in economics. In other words, bilevel programs can be considered as demand-offer equilibrium models where the demand is the result of another mathematical problem. Bilevel problems can be formulated through the generic CS model when $Y(x)$ corresponds to the optimal solutions of a mathematical program defined for a given x, i.e. $Y(x) = \operatorname{argmin}\{h(x,y)|y \in Y_2, (x,y) \in XY_2\}$ where Y_2 is defined by a set of constraints on y, and XY_2 is associated with the linking constraints.

In robust/stochastic optimization, it is assumed that the data related to a problem are subject to uncertainty. In stochastic optimization, probability distributions governing the data are known, and the objective function involves mathematical expectation(s). In robust optimization, uncertain data take value within specified sets, and the function to optimize is formulated in terms of a min-max objective typically (the solution must be optimal for the worst-case scenario). A standard modeling of uncertainty on data is obtained by defining a set of possible scenarios that can be described explicitly or implicitly. In stochastic optimization, in addition, a probability of occurrence is associated with each scenario and the expected objective value is optimized.

3.3. Solving problems with complex structures

Standard solution methods developed for CS problems solve independent sub-problems associated with each type of variables without explicitly integrating their interactions or integrating them iteratively in a heuristic way. However these subproblems are intrinsically linked and should be addressed jointly. In *mathematicaloptimization* a classical approach is to approximate the convex hull of the integer solutions of the model by its linear relaxation. The main solution methods are i) polyhedral solution methods which strengthen this linear relaxation by adding valid inequalities, ii) decomposition solution methods (Dantzig Wolfe, Lagrangian Relaxation, Benders decomposition) which aim to obtain a better approximation and solve it by generating extreme points/rays. Main challenges are i) the analysis of the strength of the cuts and their separations for polyhedral solution methods, ii) the decomposition schemes and iii) the extreme points/rays generations for the decomposition solution methods.

The main difficulty in solving *bilevel problems* is due to their non convexity and non differentiability. Even linear bilevel programs, where all functions involved are affine, are computationally challenging despite their apparent simplicity. Up to now, much research has been devoted to bilevel problems with linear or convex follower problems. In this case, the problem can be reformulated as a single-level program involving complementarity constraints, exemplifying the dual nature, continuous and combinatorial, of bilevel programs.

MISTIS Project-Team

3. Research Program

3.1. Mixture models

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

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

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

$$f(y_i; \theta) = \sum_{k=1}^{K} P(z_i = k; \theta) f(y_i \mid z_i; \theta) \ . \tag{46}$$

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

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

3.2. Markov models

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

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

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

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

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

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

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

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

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

We also consider methods which do not assume a parametric model. The approaches are non-parametric in the sense that they do not require the assumption of a prior model on the unknown quantities. This property is important since, for image applications for instance, it is very difficult to introduce sufficiently general parametric models because of the wide variety of image contents. Projection methods are then a way to decompose the unknown quantity on a set of functions (*e.g.* wavelets). Kernel methods which rely on smoothing the data using a set of kernels (usually probability distributions) are other examples. Relationships exist between these methods and learning techniques using Support Vector Machine (SVM) as this appears in the context of *level-sets estimation* (see section 3.3.2). Such non-parametric methods have become the cornerstone when dealing with functional data [77]. This is the case, for instance, when observations are curves. They enable us to model the data without a discretization step. More generally, these techniques are of great use for *dimension reduction* purposes (section 3.3.3). They enable reduction of the dimension of the functional or multivariate data without assumptions on the observations distribution. Semi-parametric methods refer to methods that include both parametric and non-parametric aspects. Examples include the Sliced Inverse Regression (SIR) method [79] which combines non-parametric regression techniques with parametric dimension reduction aspects. This is also the case in *extreme value analysis* [76], which is based on the modelling of distribution tails (see section 3.3.1). It differs from traditional statistics which focuses on the central part of distributions, *i.e.* on the most probable events. Extreme value theory shows that distribution tails can be modelled by both a functional part and a real parameter, the extreme value index.

3.3.1. Modelling extremal events

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

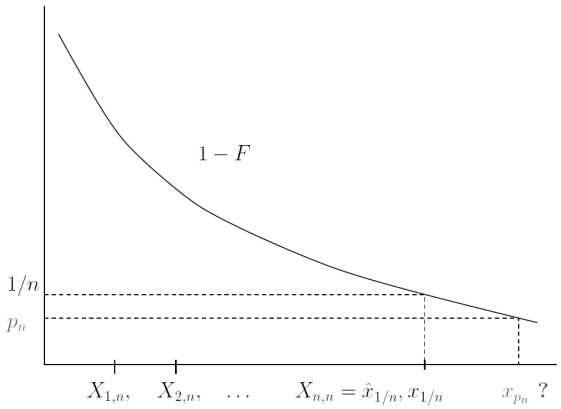

Figure 1. The curve represents the survival function $x \to P(X > x)$. The $1/n$-quantile is estimated by the maximum observation so that $\widehat{x}_{1/n} = X_{n,n}$. As illustrated in the figure, to estimate p_n-quantiles with $p_n < 1/n$, it is necessary to extrapolate beyond the maximum observation.

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

$$P(X > x) = x^{-1/\theta}\ell(x),\ x > x_0 > 0, \tag{47}$$

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

$$\frac{\ell(tx)}{\ell(x)} \to 1 \text{ as } x \to \infty \tag{48}$$

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:

$$P(X > x) = \exp\{-x^{\theta}\ell(x)\},\ x > x_0 > 0. \tag{49}$$

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

3.3.2. Level sets estimation

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

3.3.3. Dimension reduction

Our work on high dimensional data requires that we face the curse of dimensionality phenomenon. Indeed, the modelling of high dimensional data requires complex models and thus the estimation of high number of parameters compared to the sample size. In this framework, dimension reduction methods aim at replacing the original variables by a small number of linear combinations with as small as a possible loss of information. Principal Component Analysis (PCA) is the most widely used method to reduce dimension in data. However, standard linear PCA can be quite inefficient on image data where even simple image distortions can lead to highly non-linear data. Two directions are investigated. First, non-linear PCAs can be proposed, leading to semi-parametric dimension reduction methods [78]. Another field of investigation is to take into account the application goal in the dimension reduction step. One of our approaches is therefore to develop new Gaussian models of high dimensional data for parametric inference [75]. Such models can then be used in a Mixtures or Markov framework for classification purposes. Another approach consists in combining dimension reduction, regularization techniques, and regression techniques to improve the Sliced Inverse Regression method [79].

MODAL Project-Team

3. Research Program

3.1. Research axis 1: Unsupervised learning

Scientific locks related to unsupervised learning are numerous, concerning the clustering outcome validity, the ability to manage different kinds of data, the missing data questioning, the dimensionality of the data set, ... Many of them are addressed by the team, leading to publication achievements, often with a specific package delivery (sometimes upgraded as a software or even as a platform grouping several software). Because of the variety of the scope, it involves nearly all the permanent team members, often with PhD students and some engineers. The related works are always embedded inside a probabilistic framework, typically model-based approaches but also model-free ones like PAC-Bayes (PAC stands for Probably Approximately Correct), because such a mathematical environment offers both a well-posed problem and a rigorous answer.

3.2. Research axis 2: Performance assessment

One main concern of the Modal team is to provide theoretical justifications on the procedures which are designed. Such guarantees are important to avoid misleading conclusions resulting from any unsuitable use. The main ingredient in proving these guarantees is the use of the PAC framework, leading to finite-sample concentration inequalities. More precisely, contributions to PAC learning rely on the classical empirical process theory and the PAC-Bayesian theory. The Modal team exploits these non-asymptotic tools to analyze the performance of iterative algorithms (such as gradient descent), cross-validation estimators, online change-point detection procedures, ranking algorithms, matrix factorization techniques and clustering methods, for instance. The team also develops some expertise on the formal dynamic study of algorithms related to mixture models (important models used in the previous unsupervised setting), like degeneracy for EM algorithm or also label switching for Gibbs algorithm.

3.3. Research axis 3: Functional data

Mainly due to technological advances, functional data are more and more widespread in many application domains. Functional data analysis (FDA) is concerned with the modeling of data, such as curves, shapes, images or a more complex mathematical object, though as smooth realizations of a stochastic process (an infinite dimensional data object valued in a space of eventually infinite dimension; space of squared integrable functions, ...). Time series are an emblematic example even if it should not be limited to them (spectral data, spatial data, ...). Basically, FDA considers that data correspond to realizations of stochastic processes, usually assumed to be in a metric, semi-metric, Hilbert or Banach space. One may consider, functional independent or dependent (in time or space) data objects of different types (qualitative, quantitative, ordinal, multivariate, time-dependent, spatial-dependent, ...). The last decade saw a dynamic literature on parametric or non-parametric FDA approaches for different types of data and applications to various domains, such as principal component analysis, clustering, regression and prediction.

3.4. Research axis 4: Applications motivating research

The fourth axis consists in translating real application issues into statistical problems raising new (academic) challenges for models developed in Modal team. Cifre Phds in industry and interdisciplinary projects with research teams in Health and Biology are at the core of this objective. The main originality of this objective lies in the use of statistics with complex data, including in particular ultra-high dimension problems. We focus on real applications which cannot be solved by classical data analysis.

RANDOPT Team

3. Research Program

3.1. Introduction

The lines of research we intend to pursue is organized along four axis namely developing novel theoretical framework, developing novel algorithms, setting novel standards in scientific experimentation and benchmarking and applications.

3.2. Developing Novel Theoretical Frameworks for Analyzing and Designing Adaptive Stochastic Algorithms

Stochastic black-box algorithms typically optimize **non-convex, non-smooth functions**. This is possible because the algorithms rely on weak mathematical properties of the underlying functions: the algorithms do not use the derivatives—hence the function does not need to be differentiable—and, additionally, often do not use the exact function value but instead how the objective function ranks candidate solutions (such methods are sometimes called function-value-free).(To illustrate a comparison-based update, consider an algorithm that samples λ (with λ an even integer) candidate solutions from a multivariate normal distribution. Let $x_1, ..., x_\lambda$ in $\mathbb{R}^n$ denote those λ candidate solutions at a given iteration. The solutions are evaluated on the function f to be minimized and ranked from the best to the worse:

$$f(x_{1:\lambda}) \leq ... \leq f(x_{\lambda:\lambda}) \ .$$

In the previous equation $i:\lambda$ denotes the index of the sampled solution associated to the i-th best solution. The new mean of the Gaussian vector from which new solutions will be sampled at the next iteration can be updated as

$$m \longleftarrow \frac{1}{\lambda} \sum_{i=1}^{\lambda/2} x_{i:\lambda} \ .$$

The previous update moves the mean towards the $\lambda/2$ best solutions. Yet the update is only based on the ranking of the candidate solutions such that the update is the same if f is optimized or $g \circ f$ where $g : \mathrm{Im}(f) \to \mathbb{R}$ is strictly increasing. Consequently, such algorithms are invariant with respect to strictly increasing transformations of the objective function. This entails that they are robust and their performances generalize well.)

Additionally, adaptive stochastic optimization algorithms typically have a **complex state space** which encodes the parameters of a probability distribution (e.g. mean and covariance matrix of a Gaussian vector) and other state vectors. This state-space is a **manifold**. While the algorithms are Markov chains, the complexity of the state-space makes that **standard Markov chain theory tools do not directly apply**. The same holds with tools stemming from stochastic approximation theory or Ordinary Differential Equation (ODE) theory where it is usually assumed that the underlying ODE (obtained by proper averaging and limit for learning rate to zero) has its critical points inside the search space. In contrast, in the cases we are interested in, the **critical points of the ODEs are at the boundary of the domain**.

Last, since we aim at developing theory that on the one hand allows to analyze the main properties of state-of-the-art methods and on the other hand is useful for algorithm design, we need to be careful not to use simplifications that would allow a proof to be done but would not capture the important properties of the algorithms. With that respect one tricky point is to develop **theory that accounts for invariance properties**.

To face those specific challenges, we need to develop novel theoretical frameworks exploiting invariance properties and accounting for peculiar state-spaces. Those frameworks should allow researchers to analyze one of the core properties of adaptive stochastic methods, namely **linear convergence** on the widest possible class of functions.

We are planning to approach the question of linear convergence from three different complementary angles, using three different frameworks:

- the Markov chain framework where the convergence derives from the analysis of the stability of a normalized Markov chain existing on scaling-invariant functions for translation and scale-invariant algorithms [16]. This framework allows for a fine analysis where the exact convergence rate can be given as an implicit function of the invariant measure of the normalized Markov chain. Yet it requires the objective function to be scaling-invariant. The stability analysis can be particularly tricky as the Markov chain that needs to be studied writes as $\Phi_{t+1} = F(\Phi_t, W_{t+1})$ where $\{W_t : t > 0\}$ are independent identically distributed and F is typically discontinuous because the algorithms studied are comparison-based. This implies that practical tools for analyzing a standard property like irreducibility, that rely on investigating the stability of underlying deterministic control models [34], cannot be used. Additionally, the construction of a drift to prove ergodicity is particularly delicate when the state space includes a (normalized) covariance matrix as it is the case for analyzing the CMA-ES algorithm.
- The stochastic approximation or ODE framework. Those are standard techniques to prove the convergence of stochastic algorithms when an algorithm can be expressed as a stochastic approximation of the solution of a mean field ODE [19], [20], [31]. What is specific and induces difficulties for the algorithms we aim at analyzing is the **non-standard state-space** since the ODE variables correspond to the state-variables of the algorithm (e.g. $\mathbb{R}^n \times \mathbb{R}_{>0}$ for step-size adaptive algorithms, $\mathbb{R}^n \times \mathbb{R}_{>0} \times S^n_{++}$ where S^n_{++} denotes the set of positive definite matrices if a covariance matrix is additionally adapted). Consequently, the ODE can have many critical points at the boundary of its definition domain (e.g. all points corresponding to $\sigma_t = 0$ are critical points of the ODE) which is not typical. Also we aim at proving **linear convergence**, for that it is crucial that the learning rate does not decrease to zero which is non-standard in ODE method.
- The direct framework where we construct a global Lyapunov function for the original algorithm from which we deduce bounds on the hitting time to reach an ϵ-ball of the optimum. For this framework as for the ODE framework, we expect that the class of functions where we can prove linear convergence are composite of $g \circ f$ where f is differentiable and $g : \mathrm{Im}(f) \to \mathbb{R}$ is strictly increasing and that we can show convergence to a local minimum.

We expect those frameworks to be complementary in the sense that the assumptions required are different. Typically, the ODE framework should allow for proofs under the assumptions that learning rates are small enough while it is not needed for the Markov chain framework. Hence this latter framework captures better the real dynamics of the algorithm, yet under the assumption of scaling-invariance of the objective functions. Also, we expect some overlap in terms of function classes that can be studied by the different frameworks (typically convex-quadratic functions should be encompassed in the three frameworks). By studying the different frameworks in parallel, we expect to gain synergies and possibly understand what is the most promising approach for solving the holy grail question of the linear convergence of CMA-ES. We foresee for instance that similar approaches like the use of Foster-Lyapunov drift conditions are needed in all the frameworks and that intuition can be gained on how to establish the conditions from one framework to another one.

3.3. Algorithmic developments

We are planning on developing algorithms in the subdomains with strong practical demand for better methods of constrained, multiobjective, large-scale and expensive optimization.

Many of the algorithm developments, we propose, rely on the CMA-ES method. While this seems to restrict our possibilities, we want to emphasize that CMA-ES became a *family of methods* over the years that nowadays include various techniques and developments from the literature to handle non-standard optimization problems (noisy, large-scale, ...). The core idea of all CMA-ES variants—namely the mechanism to adapt a Gaussian distribution—has furthermore been shown to derive naturally from first principles with only minimal assumptions in the context of derivative-free black-box stochastic optimization [35], [24]. This is a strong justification for relying on the CMA-ES premises while new developments naturally include new techniques typically borrowed from other fields. While CMA-ES is now a full family of methods, for visibility reasons, we continue to refer often to "the CMA-ES algorithm".

3.3.1. Constrained optimization

Many (real-world) optimization problems have constraints related to technical feasibility, cost, etc. Constraints are classically handled in the black-box setting either via rejection of solutions violating the constraints—which can be quite costly and even lead to quasi-infinite loops—or by penalization with respect to the distance to the feasible domain (if this information can be extracted) or with respect to the constraint function value [21]. However, the penalization coefficient is a sensitive parameter that needs to be adapted in order to achieve a robust and general method [22]. Yet, **the question of how to handle properly constraints is largely unsolved**. The latest constraints handling for CMA-ES is an ad-hoc technique driven by many heuristics [22]. Also, it is particularly only recently that it was pointed out that **linear convergence properties should be preserved** when addressing constraint problems [14].

Promising approaches though, rely on using augmented Lagrangians [14], [15]. The augmented Lagrangian, here, is the objective function optimized by the algorithm. Yet, it depends on coefficients that are adapted online. The adaptation of those coefficients is the difficult part: the algorithm should be stable and the adaptation efficient. We believe that the theoretical frameworks developed (particularly the Markov chain framework) will be useful to understand how to design the adaptation mechanisms. Additionally, the question of invariance will also be at the core of the design of the methods: augmented Lagrangian approaches break the invariance to monotonic transformation of the objective functions, yet understanding the maximal invariance that can be achieved seems to be an important step towards understanding what adaptation rules should satisfy.

3.3.2. Large-scale Optimization

In the large-scale setting, we are interested to optimize problems with the order of 10^3 to 10^4 variables. For one to two orders of magnitude more variables, we will talk about a “very large-scale" setting.

In this context, algorithms with a quadratic scaling (internal and in terms of number of function evaluations needed to optimize the problem) cannot be afforded. In CMA-ES-type algorithms, we typically need to restrict the model of the covariance matrix to have only a linear number of parameters to learn such that the algorithms scale linearly in terms of internal complexity, memory and number of function evaluations to solve the problem. The main challenge is thus to have rich enough models for which we can efficiently design proper adaptation mechanisms. Some first large-scale variants of CMA-ES have been derived. They include the online adaptation of the complexity of the model [13], [12]. Yet so far they fail to optimize functions whose Hessian matrix has some small eigenvalues (say around 10^{-4}) some eigenvalues equal to 1 and some very large eigenvalue (say around 10^4), that is functions whose level sets have short and long axis.

Another direction, we want to pursue, is exploring the use of large-scale variants of CMA-ES to solve reinforcement learning problems [36].

Last, we are interested to investigate the very-large-scale setting. One approach consists in doing optimization in subspaces. This entails the efficient identification of relevant spaces and the restriction of the optimization to those subspaces.

3.3.3. Multiobjective Optimization

Multiobjective optimization, i.e., the simultaneous optimization of multiple objective functions, differs from single-objective optimization in particular in its optimization goal. Instead of aiming at converging to the

solution with the best possible function value, in multiobjective optimization, a set of solutions [0] is sought. This set, called Pareto-set, contains all trade-off solutions in the sense of Pareto-optimality—no solution exists that is better in *all* objectives than a Pareto-optimal one. Because converging towards a set differs from converging to a single solution, it is no surprise that we might lose many good convergence properties if we directly apply search operators from single-objective methods. However, this is what has typically been done so far in the literature. Indeed, most of the research in stochastic algorithms for multiobjective optimization focused instead on the so called selection part, that decides which solutions should be kept during the optimization—a question that can be considered as solved for many years in the case of single-objective stochastic adaptive methods.

We therefore aim at rethinking search operators and adaptive mechanisms to improve existing methods. We expect that we can obtain orders of magnitude better convergence rates for certain problem types if we choose the right search operators. We typically see two angles of attack: On the one hand, we will study methods based on scalarizing functions that transform the multiobjective problem into a set of single-objective problems. Those single-objective problems can then be solved with state-of-the-art single-objective algorithms. Classical methods for multiobjective optimization fall into this category, but they all solve multiple single-objective problems subsequently (from scratch) instead of dynamically changing the scalarizing function during the search. On the other hand, we will improve on currently available population-based methods such as the first multiobjective versions of the CMA-ES. Here, research is needed on an even more fundamental level such as trying to understand success probabilities observed during an optimization run or how we can introduce non-elitist selection (the state of the art in single-objective stochastic adaptive algorithms) to increase robustness regarding noisy evaluations or multi-modality. The challenge here, compared to single-objective algorithms, is that the quality of a solution is not anymore independent from other sampled solutions, but can potentially depend on all known solutions (in the case of three or more objective functions), resulting in a more noisy evaluation as the relatively simple function-value-based ranking within single-objective optimizers.

3.3.4. Expensive Optimization

In the so-called expensive optimization scenario, a single function evaluation might take several minutes or even hours in a practical setting. Hence, the available budget in terms of number of function evaluation calls to find a solution is very limited in practice. To tackle such expensive optimization problems, it is needed to exploit the first few function evaluations in the best way. To this end, typical methods couple the learning of a surrogate (or meta-model) of the expensive objective function with traditional optimization algorithms.

In the context of expensive optimization and CMA-ES, which usually shows its full potential when the number n of variables is not too small (say larger than 3) and if the number of available function evaluations is about $100n$ or larger, several research directions emerge. The two main possibilities to integrate meta-models into the search with CMA-ES type algorithms are (i) the successive injection of the minimum of a learned meta-model at each time step into the learning of CMA-ES's covariance matrix and (ii) the use of a meta-model to predict the internal ranking of solutions. While for the latter, first results exist, the former idea is entirely unexplored for now. In both cases, a fundamental question is which type of meta-model (linear, quadratic, Gaussian Process, ...) is the best choice for a given number of function evaluations (as low as one or two function evaluations) and at which time the type of the meta-model shall be switched.

3.4. Setting novel standards in scientific experimentation and benchmarking

Numerical experimentation is needed as a complement to theory to test novel ideas, hypotheses, the stability of an algorithm, and/or to obtain quantitative estimates. Optimally, theory and experimentation go hand in hand, jointly guiding the understanding of the mechanisms underlying optimization algorithms. Though performing numerical experimentation on optimization algorithms is crucial and a common task, it is non-trivial and easy to fall in (common) pitfalls as stated by J. N. Hooker in his seminal paper [26].

In the RandOpt team we aim at raising the standards for both scientific experimentation and benchmarking.

[0] Often, this set forms a manifold of dimension one smaller than the number of objectives.

On the experimentation aspect, we are convinced that there is common ground over how scientific experimentation should be done across many (sub-)domains of optimization, in particular with respect to the visualization of results, testing extreme scenarios (parameter settings, initial conditions, etc.), how to conduct understandable and small experiments, how to account for invariance properties, performing scaling up experiments and so forth. We therefore want to formalize and generalize these ideas in order to make them known to the entire optimization community with the final aim that they become standards for experimental research.

Extensive numerical benchmarking, on the other hand, is a compulsory task for evaluating and comparing the performance of algorithms. It puts algorithms to a standardized test and allows to make recommendations which algorithms should be used preferably in practice. To ease this part of optimization research, we have been developing the Comparing Continuous Optimizers platform (COCO) since 2007 which allows to automatize the tedious task of benchmarking. It is a game changer in the sense that the freed time can now be spent on the scientific part of algorithm design (instead of implementing the experiments, visualization, statistical tests, etc.) and it opened novel perspectives in algorithm testing. COCO implements a thorough, well-documented methodology that is based on the above mentioned general principles for scientific experimentation.

Also due to the freely available data from 200+ algorithms benchmarked with the platform, COCO became a quasi-standard for single-objective, noiseless optimization benchmarking. It is therefore natural to extend the reach of COCO towards other subdomains (particularly constrained optimization, many-objective optimization) which can benefit greatly from an automated benchmarking methodology and standardized tests without (much) effort. This entails particularly the design of novel test suites and rethinking the methodology for measuring performance and more generally evaluating the algorithms. Particularly challenging is the design of scalable non-trivial testbeds for constrained optimization where one can still control where the solutions lies. Other optimization problem types, we are targeting are expensive problems (and the Bayesian optimization community in particular, see our AESOP project), optimization problems in machine learning (for example parameter tuning in reinforcement learning), and the collection of real-world problems from industry.

Another aspect of our future research on benchmarking is to investigate the large amounts of benchmarking data, we collected with COCO during the years. Extracting information about the influence of algorithms on the best performing portfolio, clustering algorithms of similar performance, or the automated detection of anomalies in terms of good/bad behavior of algorithms on a subset of the functions or dimensions are some of the ideas here.

Last, we want to expand the focus of COCO from automatized (large) benchmarking experiments towards everyday experimentation, for example by allowing the user to visually investigate algorithm internals on the fly or by simplifying the set up of algorithm parameter influence studies.

REALOPT Project-Team

3. Research Program

3.1. Introduction

Integer Programming Graph Theory Decomposition Approaches Polyhedral Approaches Quadratic Programming Approaches constraint programming.

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, decomposition and reformulation techniques in 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, High Performance and Cloud Computing.

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 [58]. 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 variable fixing techniques, 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, ...). Such methods are likely to produce good quality solutions only if the integer programming formulation is of top quality, i.e., if its LP relaxation provides a good approximation of the IP solution.

In the same line, variable fixing techniques, that are essential in reducing the size of large scale problems, rely on good quality approximations: either tight formulations or tight relaxation solvers (as a dynamic program combined with state space relaxation). Then if the dual bound derives when the variable is fixed to one exceeds the incubent solution value, the variable can be fixed to zero and hence removed from the problem. The process can be apply sequentially by refining the degree of relaxation.

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. Approximation Algorithms

In some contexts, obtaining an exact solution to an optimization problem is not feasible: when instances are too large, or when decisions need to be taken rapidly. Since most of the combinatorial optimization problems are NP-hard, another direction to obtain good quality solutions in reasonable time is to focus on **approximation algorithms**. The definition of approximation algorithms is based on the notion of input set $\mathcal{I}$ and each $I \in \mathcal{I}$ defines a solution space $\mathcal{S}_I$. For a minimization problem $\min_{x \in \mathcal{S}_I} f(x)$, an algorithm $\mathcal{A}$ is an α-approximation algorithm if it provides a solution within α of the optimal solution for all instances in the input set:

$$\forall I \in \mathcal{I}, \quad f(\mathcal{A}(I)) \leq \alpha \min_{x \in \mathcal{S}_I} f(x) = f^*(I)$$

The objective is to search for polynomial algorithms, with approximation ratios as close to 1 as possible. Such algorithms are called *worst-case* approximation algorithms, because the performance guarantee is expressed over all possible inputs of the problem. The design of these algorithms have strong links with the enumeration techniques described above: since computing $f^*(I)$ is an NP-hard problem, it is often required to derive **strong a priori bounds** on the optimal solution value which can afterward be compared to estimations of the value of the solution produced. In many cases, it is also possible to build α-approximate solutions by a careful rounding of a solution obtained from the linear relaxation of an integer formulation of the problem. Members of the team have expertise in designing and evaluating approximation algorithms for resource allocation in computer systems, using a variety of techniques, such as dual approximation (where a guess of the optimal value f^* is provided, and $\mathcal{A}$ either provides a solution within αf^*, or guarantees that no solution of value f^* or less exists), or resource augmentation (where an approximation is obtained by relaxing some of the constraints of the problem).

3.7. Polyhedral Combinatorics and Graph Theory

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

SELECT Project-Team

3. Research Program

3.1. General presentation

From applications we treat on a day-to-day basis, we have learned that some assumptions currently used in asymptotic theory for model selection are often irrelevant in practice. For instance, it is not realistic to assume that the target belongs to the family of models in competition. Moreover, in many situations, it is useful to make the size of the model depend on the sample size, which makes asymptotic analyses breakdown. An important aim of SELECT is to propose model selection criteria which take such practical constraints into account.

3.2. A nonasymptotic view of model selection

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

3.3. Taking into account the modeling purpose in model selection

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

3.4. Bayesian model selection

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

SEQUEL Project-Team

3. Research Program

3.1. In Short

SEQUEL is primarily grounded on two domains:

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

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

3.2. Decision-making Under Uncertainty

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

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

3.2.1. Reinforcement Learning

Sequential decision processes occupy the heart of the SEQUEL project; a detailed presentation of this problem may be found in Puterman's book [60].

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

In the MDP $(\mathcal{X}, \mathcal{A}, P, r)$, each initial state x_0 and action sequence $a_0, a_1, ...$ gives rise to a sequence of states $x_1, x_2, ...$, satisfying $\mathbb{P}(x_{t+1} = x'|x_t = x, a_t = a) = p(x'|x, a)$, 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:

$$V^\pi(x) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t | x_0 = x, \pi\right], \tag{50}$$

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 [59]) 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) [57], 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 [58]. 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 $x \in \mathcal{X}$,

$$V^*(x) = \max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V^*(x')\right]. \tag{51}$$

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:

$$\pi^*(x) \in \arg\max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V^*(x')\right]. \tag{52}$$

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 ([63]):

- 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 [61], 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.* [56] 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 behavior (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 behavior, or than a class of other behaviors.

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 piece-wise 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) behavior 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 $x^1 = (x^1_1, \cdots, x^1_{n_1}), \cdots, x^N = (x^1_N, \cdots, x^N_{n_N})$, we wish to group similar objects together. While this is of course not a precise formulation, it can be made precise if we assume that the samples were generated by k different distributions.

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

3.3.5. Online Semi-Supervised Learning

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

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

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

3.3.6. Online Kernel and Graph-Based Methods

Large-scale kernel ridge regression is limited by the need to store a large kernel matrix. Similarly, large-scale graph-based learning is limited by storing the graph Laplacian. Furthermore, if the data come online, at some point no finite storage is sufficient and per step operations become slow.

Our challenge is to design sparsification methods that give guaranteed approximate solutions with a reduced storage requirements.

SIERRA Project-Team

3. Research Program

3.1. Supervised Learning

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

3.2. Unsupervised Learning

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

3.3. Parsimony

The concept of parsimony is central to many areas of science. In the context of statistical machine learning, this takes the form of variable or feature selection. The team focuses primarily on structured sparsity, with theoretical and algorithmic contributions.

3.4. Optimization

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

TAU Team

3. Research Program

3.1. Toward Good AI

As discussed by [134], the topic of ethical AI was non-existent until 2010, was laughed at in 2016, and became a hot topic in 2017 as the AI disruptivity with respect to the fabric of life (travel, education, entertainment, social networks, politics, to name a few) became unescapable [131], together with its expected impacts on the nature and amount of jobs. As of now, it seems that the risk of a new AI Winter might arise from legal[0] and societal[0] issues. While privacy is now recognized as a civil right in Europe, it is feared that the GAFAM, BATX and others can already capture a sufficient fraction of human preferences and their dynamics to achieve their commercial and other goals, and build a Brave New Big Brother (BNBB, a system that is openly beneficial to many, covertly nudging, and possibly dictatorial).

The ambition of TAU is to mitigate the BNBB risk along several intricated dimensions, and build i) causal and explainable models; ii) fair data and models; iii) provably robust models.

3.1.1. Causal modeling and biases

Participants: Isabelle Guyon, Michèle Sebag, Philippe Caillou, Paola Tubaro
PhD: Diviyan Kalainathan
Collaboration: Olivier Goudet (TAU then Univ. Angers), David Lopez-Paz (Facebook)

The extraction of causal models, a long goal of AI [132], [112], [133], became a strategic issue as the usage of learned models gradually shifted from *prediction* to *prescription* in the last years. This evolution, following Auguste Comte's vision of science (*Savoir pour prévoir, afin de pouvoir*) indeed reflects the exuberant optimism about AI: Knowledge enables Prediction; Prediction enables Control. However, although predictive models can be based on correlations, prescriptions can only be based on causal models[0].

Among the research applications concerned with causal modeling, predictive modeling or collaborative filtering at TAU are all projects described in section 4.1 (see also Section 3.4), studying the relationships between: i) the educational background of persons and the job openings (FUI project JobAgile and DataIA project Vadore); ii) the quality of life at work and the economic performance indicators of the enterprises (ISN Lidex project Amiqap) [114] ; iii) the nutritional items bought by households (at the level of granularity of the barcode) and their health status, as approximated from their body-mass-index (IRS UPSaclay Nutriperso); iv) the actual offer of restaurants and their scores on online rating systems. In these projects, a wealth of data is available (though hardly sufficient for applications ii), iii and iv))) and there is little doubt that these data reflect the imbalances and biases of the world as is, ranging from gender to racial to economical prejudices. Preventing the learned models from perpetuating such biases is essential to deliver an AI endowed with common decency.

In some cases, the bias is known; for instance, the cohorts in the Nutriperso study are more well-off than the average French population, and the Kantar database includes explicit weights to address this bias through importance sampling. In other cases, the bias is only guessed; for instance, the companies for which Secafi data are available hardly correspond to a uniform sample as these data have been gathered upon the request of the company trade union.

[0]For instance, the (fictitious) plea challenge proposed to law students in Oct. 2018 considered a chain reaction pileup occurred among autonomous and humanly operated vehicles on a highway.

[0]For instance related to information bubbles and nudge [98], [148].

[0]One can predict that it rains based on the presence of umbrellas in the street; but one cannot induce rainfall by going out with an umbrella. Likewise, the presence of books/tablets at home and the good scores of children at school are correlated; but offering books/tablets to all children might fail to improve their scores *per se*, if both good scores and books are explained by a so-called confounder variable, like the presence of adults versed in books/tablets at home.

3.1.2. Robustness of Learned Models

Participants: Guillaume Charpiat, Marc Schoenauer, Michèle Sebag
PhD and Engineers: Julien Girard, Marc Nabhan, Nizham Makhoud, Raphaël Jaiswal
Collaboration: Zakarian Chihani (CEA); Hiba Hage, Philippe Reynaud, and Yves Tourbier (Renault)

Due to their outstanding performances, deep neural networks and more generally machine learning-based decision making systems, referred to as MLs in the following, have been raising hopes in the recent years to achieve breakthroughs in critical systems, ranging from autonomous vehicles to defense. The main pitfall for such applications lies in the lack of guarantees for MLs robustness.

Specifically, MLs are used when the mainstream software design process does not apply, that is, when no formal specification of the target software behavior is available and/or when the system is embedded in an open unpredictable world. The extensive body of knowledge developed to deliver guarantees about mainstream software – ranging from formal verification, model checking and abstract interpretation to testing, simulation and monitoring – thus does not directly apply either. Another weakness of MLs regards their dependency to the amount and quality of the training data, as their performances are sensitive to slight perturbations of the data distribution. Such perturbations can occur naturally due to domain or concept drift (e.g. due to a change in light intensity or a scratch on a camera lens); they can also result from intentional malicious attacks, a.k.a adversarial examples [149].

These downsides, currently preventing the dissemination of MLs in safety-critical systems (SCS), call for a considerable amount of research, in order to understand when and to which extent an MLs can be certified to provide the desired level of guarantees.

Julien Girard's PhD (CEA scholarship), started in Oct. 2018, co-supervised by Guillaume Charpiat and Zakaria Chihani (CEA), is devoted to the extension of abstract interpretation to deep neural nets, and the formal characterization of the transition kernel from input to output space achieved by a DNN (robustness by design, coupled with formally assessing the coverage of the training set). This approach is tightly related to the inspection and opening of black-box models, aimed to characterize the patterns in the input instances responsible for a decision – another step toward explainability.

On the other hand, experimental validation of MLs, akin statistical testing, also faces three limitations: i) real-world examples are notoriously insufficient to ensure a good coverage in general; ii) for this reason, simulated examples are extensively used; but their use raises the *reality gap* issue [123] of the distance between real and simulated worlds; iii) independently, the real-world is naturally subject to domain shift (e.g. due to the technical improvement and/or aging of sensors). Our collaborations with Renault tackle such issues in the context of the autonomous vehicle (see Section 7.1.3).

3.2. Hybridizing numerical modeling and learning systems

Participants: Guillaume Charpiat, Cécile Germain, Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhD: Théophile Sanchez, Loris Felardo
In sciences and engineering, human knowledge is commonly expressed in closed form, through equations or mechanistic models characterizing how a natural or social phenomenon, or a physical device, will behave/evolve depending on its environment and external stimuli, under some assumptions and up to some approximations. The field of numerical engineering, and the simulators based on such mechanistic models, are at the core of most approaches to understand and analyze the world, from solid mechanics to computational fluid dynamics, from chemistry to molecular biology, from astronomy to population dynamics, from epidemiology and information propagation in social networks to economy and finance.

Most generally, numerical engineering supports the simulation, and when appropriate the optimization and control[0] of the phenomenons under study, although several sources of discrepancy might adversely affect the results, ranging from the underlying assumptions and simplifying hypotheses in the models, to systematic experiment errors to statistical measurement errors (not to mention numerical issues). This knowledge and know-how are materialized in millions of lines of code, capitalizing the expertise of academic and industrial labs. These softwares have been steadily extended over decades, modeling new and more fine-grained effects through layered extensions, making them increasingly harder to maintain, extend and master. Another difficulty is that complex systems most often resort to hybrid (pluridisciplinary) models, as they involve many components interacting along several time and space scales, hampering their numerical simulation.

At the other extreme, machine learning offers the opportunity to model phenomenons from scratch, using any available data gathered through experiments or simulations. Recent successes of machine learning in computer vision, natural language processing and games to name a few, have demonstrated the power of such agnostic approaches and their efficiency in terms of prediction [118], inverse problem solving [161], and sequential decision making [154], [81], despite their lack of any "semantic" understanding of the universe. Even before these successes, Anderson's claim was that *the data deluge [might make] the scientific method obsolete* [69], as if a reasonable option might be to throw away the existing equational or software bodies of knowledge, and let Machine Learning rediscover all models from scratch. Such a claim is hampered among others by the fact that not all domains offer a wealth of data, as any academic involved in an industrial collaboration around data has discovered.

Another approach will be considered in TAU, investigating how existing mechanistic models and related simulators can be partnered with ML algorithms: i) to achieve the same goals with the same methods with a gain of accuracy or time; ii) to achieve new goals; iii) to achieve the same goals with new methods.

Toward more robust numerical engineering: In domains where satisfying mechanistic models and simulators are available, ML can contribute to improve their accuracy or usability. A first direction is to refine or extend the models and simulators to better fit the empirical evidence. The goal is to finely account for the different biases and uncertainties attached to the available knowledge and data, distinguishing the different types of *known unknowns*. Such *known unknowns* include the model hyper-parameters (coefficients), the systematic errors due to e.g., experiment imperfections, and the statistical errors due to e.g., measurement errors. A second approach is based on learning a surrogate model for the phenomenon under study that incorporate domain knowledge from the mechanistic model (or its simulation). See Section 7.5 for case studies.

A related direction, typically when considering black-box simulators, aims to learn a model of the error, or equivalently, a post-processor of the software. The discrepancy between simulated and empirical results, referred to as *reality gap* [123], can be tackled in terms of domain adaptation [74], [97]. Specifically, the source domain here corresponds to the simulated phenomenon, offering a wealth of inexpensive data, and the target domain corresponds to the actual phenomenon, with rare and expensive data; the goal is to devise accurate target models using the source data and models.

Extending numerical engineering: ML, using both experimental and numerical data, can also be used to tackle new goals, that are beyond the current state-of-the-art of standard approaches. Inverse problems are such goals, identifying the parameters or the initial conditions of phenomenons for which the model is not differentiable, or amenable to the adjoint state method.

A slightly different kind of inverse problem is that of recovering the ground truth when only noisy data is available. This problem can be formulated as a search for the simplest model explaining the data. The question then becomes to formulate and efficiently exploit such a simplicity criterion.

Another goal can be to model the distribution of given quantiles for some system: The challenge is to exploit available data to train a generative model, aimed at sampling the target quantiles.

[0]Note that the causal nature of mechanistic models is established from prior knowledge and experimentations.

Examples tackled in TAU are detailed in Section 7.5 . Note that the "Cracking the Glass Problem", described in Section 7.2.3 is yet another instance of a similar problem.

Data-driven numerical engineering : Finally, ML can also be used to sidestep numerical engineering limitations in terms of scalability, or to build a simulator emulating the resolution of the (unknown) mechanistic model from data, or to revisit the formal background.

When the mechanistic model is known and sufficiently accurate, it can be used to train a deep network on an arbitrary set of (space,time) samples, resulting in a meshless numerical approximation of the model [145], supporting by construction *differentiable programming* [120].

When no mechanistic model is sufficiently efficient, the model must be identified from the data only. Genetic programming has been used to identify systems of ODEs [142], through the identification of invariant quantities from data, as well as for the direct identification of control commands of nonlinear complex systems, including some chaotic systems [85]. Another recent approach uses two deep neural networks, one for the state of the system, the other for the equation itself [135]. The critical issues for both approaches include the scalability, and the explainability of the resulting models. Such line of research will benefit from TAU unique mixed expertise in Genetic Programming and Deep Learning.

Finally, in the realm of signal processing (SP), the question is whether and how deep networks can be used to revisit mainstream feature extraction based on Fourier decomposition, wavelet and scattering transforms [77]. E. Bartenlian's PhD (started Oct. 2018), co-supervised by M. Sebag and F. Pascal (Centrale-Supélec), focusing on musical audio-to-score translation [144], inspects the effects of supervised training, taking advantage from the fact that convolution masks can be initialized and analyzed in terms of frequency.

3.3. Learning to learn

According to Ali Rahimi's test of times award speech at NIPS 17, the current ML algorithms *have become a form of alchemy*. Competitive testing and empirical breakthroughs gradually become mandatory for a contribution to be acknowledged; an increasing part of the community adopts trials and errors as main scientific methodology, and theory is lagging behind practice. This style of progress is typical of technological and engineering revolutions for some; others ask for consolidated and well-understood theoretical advances, saving the time wasted in trying to build upon hardly reproducible results.

Basically, while practical achievements have often passed the expectations, there exist caveats along three dimensions. Firstly, excellent performances do not imply that the model has captured what was to learn, as shown by the phenomenon of adversarial examples. Following Ian Goodfellow, some well-performing models might be compared to *Clever Hans*, the horse that was able to solve mathematical exercizes using non verbal cues from its teacher [111]; it is the purpose of Pillar I. to alleviate the *Clever Hans* trap (section 3.1).
Secondly, some major advances, e.g. related to the celebrated adversarial learning [101], [97], establish proofs of concept more than a sound methodology, where the reproducibility is limited due to i) the computational power required for training (often beyond reach of academic labs); ii) the numerical instabilities (witnessed as random seeds happen to be found in the codes); iii) the insufficiently documented experimental settings. What works, why and when is still a matter of speculation, although better understanding the limitations of the current state of the art is acknowledged to be a priority. After Ali Rahimi again, *simple experiments, simple theorems are the building blocks that help us understand more complicated systems*. Along this line, [128] propose toy examples to demonstrate and understand the defaults of convergence of gradient descent adversarial learning.
Thirdly, and most importantly, the reported achievements rely on carefully tuned learning architectures and hyper-parameters. The sensitivity of the results to the selection and calibration of algorithms has been identified since the end 80s as a key ML bottleneck, and the field of automatic algorithm selection and calibration, referred to as AutoML or Auto-☆ in the following, is at the ML forefront.

TAU aims to contribute to the ML evolution toward a more mature stage along three dimensions. In the short term, the research done in Auto-☆ will be pursued (section 3.3.1). In the medium term, an information theoretic perspective will be adopted to capture the data structure and to calibrate the learning algorithm *depending on the nature and amount of the available data*. In the longer term, our goal is to leverage the methodologies forged in statistical physics to understand and control the trajectories of complex learning systems (section 3.3.3).

3.3.1. Auto-*

Participants: Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhD: Guillaume Doquet, Zhengying Liu, Herilalaina Rakotoarison, Lisheng Sun
Collaboration: Olivier Bousquet, André Elisseeff (Google Zurich)

The so-called Auto-☆ task, concerned with selecting a (quasi) optimal algorithm and its hyper-parameters depending on the problem instance at hand, remained a key issue in ML for the last three decades [75], as well as in optimization at large [110], including combinatorial optimization and constraint satisfaction [117], [100] and continuous optimization [71]. This issue, tackled by several European projects along the decades, governs the knowledge transfer to industry, due to the shortage of data scientists. It becomes even more crucial as models are more complex and their training requires more computational resources. This has motivated several international challenges devoted to Auto-ML [45] (see also Section 3.4), including the on-going AutoDL [37] (see also Section 7.6).

Several approaches have been used to tackle Auto-☆ in the literature, and TAU has been particularly active in the first two. Meta-learning aims to build a surrogate performance model, estimating the performance of an algorithm configuration on *any* problem instance characterized from its meta-feature values [138], [100], [72], [71] [11]. Collaborative filtering, considering that a problem instance "likes better" an algorithm configuration yielding a better performance, learns to recommend good algorithms to problem instances [147], [130]. Bayesian optimization proceeds by alternatively building a surrogate model of algorithm performances on *the* problem instance at hand, and tackling it [92]. This last approach currently is the prominent one; as shown in [130], the meta-features developed for AutoML are hardly relevant, hampering both meta-learning and collaborative filtering.

Beyond these, current research directions in TAU include the design of more efficient features, as well as the design of an original approach based on MCTS algorithm (see Section 7.2.1).

3.3.2. Information theory: adjusting model complexity and data fitting

Participants: Guillaume Charpiat, Marc Schoenauer, Michèle Sebag
PhD: Corentin Tallec, Pierre Wolinski, Léonard Blier
Collaboration: Yann Ollivier (Facebook)

In the 60s, Kolmogorov and Solomonoff provided a well-grounded theory for building (probabilistic) models best explaining the available data [139], [103], that is, the shortest programs able to generate these data. Such programs can then be used to generate further data or to answer specific questions (interpreted as missing values in the data). Deep learning, from this viewpoint, efficiently explores a space of computation graphs, described from its hyperparameters (network structure) and parameters (weights). Network training amounts to optimizing these parameters, namely, navigating the space of computational graphs to find a network, as simple as possible, that explain the past observations well.

This vision is at the core of variational auto-encoders [116], directly optimizing a bound on the Kolmogorov complexity of the dataset. More generally variational methods provide quantitative criteria to identify superfluous elements (edges, units) in a neural network, that can potentially be used for structural optimization of the network (Leonard Blier's PhD, started Oct. 2018).

The same principles apply to unsupervised learning, aimed to find the maximum amount of structure hidden in the data, quantified using this information-theoretic criterion.

The known invariances in the data can be exploited to guide the model design (e.g. as translation invariance leads to convolutional structures, or LSTM is shown to enforce the invariance to time affine transformations of the data sequence [150]). Scattering transforms exploit similar principles [77]. A general theory of how to detect *unknown* invariances in the data, however, is currently lacking.

The view of information theory and Kolmogorov complexity suggests that key program operations (composition, recursivity, use of predefined routines) should intervene when searching for a good computation graph. One possible framework for exploring the space of computation graphs with such operations is that of genetic programming [70]. It is interesting to see that evolutionary computation appeared in the last two years among the best candidates to explore the space of deep learning structures [137], [122]. Other approaches might proceed by combining simple models into more powerful ones, e.g. using "Context Tree Weighting" [158] or switch distributions [88]. Another option is to formulate neural architecture design as a reinforcement learning problem [73]; the value of the building blocks (predefined routines) might be defined using e.g., Monte-Carlo Tree Search. A key difficulty is the computational cost of retraining neural nets from scratch upon modifying their architecture; an option might be to use neutral initializations to support warm-restart.

3.3.3. Analyzing and Learning Complex Systems

Participants: Cyril Furtlehner, Aurélien Decelle, François Landes, Michèle Sebag
PhD: Giancarlo Fissore
Collaboration: Enrico Camporeale (CWI); Jacopo Rocchi (LPTMS Paris Sud), the Simons team: Rahul Chako (post-doc), Andrea Liu (UPenn), David Reichman (Columbia), Giulio Biroli (ENS), Olivier Dauchot (ESPCI).

Methods and criteria from statistical physics have been widely used in ML. In early days, the capacity of Hopfield networks (associative memories defined by the attractors of an energy function) was investigated by using the replica formalism [68]. Restricted Boltzmann machines likewise define a generative model built upon an energy function trained from the data. Along the same lines, Variational Auto-Encoders can be interpreted as systems relating the free energy of the distribution, the information about the data and the entropy (the degree of ignorance about the micro-states of the system) [157]. A key promise of the statistical physics perspective and the Bayesian view of deep learning is to harness the tremendous growth of the model size (billions of weights in recent machine translation netwowrks), and make them sustainable through e.g. weight quantization [125], posterior drop-out [129], and probabilistic binary networks [126]. Such "informational cooling" of a trained deep network can reduce its size by several orders of magnitude while preserving its performance.

Statistical physics is among the key expertises of TAU, originally only represented by Cyril Furtlehner, later strenghtened by Aurélien Decelle's and François Landes' arrivals in 2014 and 2018. On-going studies are conducted along several directions.

Generative models are most often expressed in terms of a Gibbs distributions $P[S] = \exp(-E[S])$, where energy E involves a sum of building blocks, modelling the interactions among variables. This formalization makes it natural to use mean-field methods of statistical physics and associated inference algorithms to both train and exploit such models. The difficulty is to find a good trade-off between the richness of the structure and the efficiency of mean-field approaches. One direction of research pursued in TAU, [94] in the context of traffic forecasting, is to account for the presence of cycles in the interaction graph, to adapt inference algorithms to such graphs with cycles, while constraining graphs to remain compatible with mean-field inference.

Another direction, explored in TAO in the recent years, is based on the definition and exploitation of self-consistency properties, enforcing principled divide-and-conquer resolutions. In the particular case of the message-passing Affinity Propagation algorithm for instance [159], self-consistency imposes the invariance of the solution when handled at different scales, thus enabling to characterize the critical value of the penalty and other hyper-parameters in closed form (in the case of simple data distributions) or empirically otherwise [95].

A more recent research direction examines the quantity of information in a (deep) neural net along the random matrix theory framework [80]. It is addressed in Giancarlo Fissore's PhD, and is detailed in Section 7.2.3 .

A collaboration with L. Zbederova's group at Ecole Normale Supérieure is just starting, thanks to François Landes' arrival, based on the study of some information-theoretic indicators for some class of Neural Network. It is, too, described in more details in Section 7.2.3 .

Finally, we note the recent surge in using ML to address fundamental physics problems: from turbulence to high-energy physics and soft matter as well (with glasses at its core). TAU's dual expertise in Deep Networks and in statistical physics places it in an ideal position to significantly contribute to this domain and shape the methods that will be used by the physics community in the future. François Landes' recent arrival in the team makes TAU a unique place for such interdisciplinary research, thanks to his collaborators from the Simons Collaboration *Cracking the Glass Problem* (gathering 13 statistical physics teams at the international level). This project is detailed in Section 7.2.3 .

3.4. Organisation of Challenges

Participants: Cécile Germain, Isabelle Guyon, Marc Schoenauer, Michèle Sebag
Challenges have been an important drive for Machine Learning research for many years, and TAO members have played important roles in the organization of many such challenges: Michèle Sebag was head of the challenge programme in the Pascal European Network of Excellence (2005-2013); Isabelle Guyon, as mentioned, was the PI of many challenges ranging from causation challenges [104], to AutoML [105]. The Higgs challenge [65], most attended ever Kaggle challenge, was jointly organized by TAO (C. Germain), LAL-IN2P3 (D. Rousseau and B. Kegl) and I. Guyon (not yet at TAO), in collaboration with CERN and Imperial College.

TAU was also particularly implicated with the ChaLearn Looking At People (LAP) challenge series in Computer Vision, in collaboration with the University of Barcelona [90] including the Job Candidate Screening Coopetition [89]; the Real Versus Fake Expressed Emotion Challenge (ICCV 2017) [155]; the Large-scale Continuous Gesture Recognition Challenge (ICCV 2017) [155]; the Large-scale Isolated Gesture Recognition Challenge (ICCV 2017) [155].

Other challenges have been organized in 2018, or are planned for the near future, detailed in Section 7.6 . In particular, many of them now run on the Codalab platform, managed by TAU and maintained at LRI.

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. The team CQFD focuses on two complementary types of approaches. The first approach is based on mathematical representations built upon physical models where the dynamic of the real system is described by *stochastic processes*. The second one consists in studying the modeling issue in an abstract framework where the real system is considered as black-box. In this context, the outputs of the system are related to its inputs through a *statistical model*. Regarding stochastic processes, the team studies Piecewise Deterministic Markov Processes (PDMPs) and Markov Decision Processes (MDPs). These two classes of Markov processes form general families of controlled stochastic models suitable for the design of sequential decision-making problems. They appear in many fields such as biology, engineering, computer science, economics, operations research and provide powerful classes of processes for the modeling of complex systems. Our contribution to this topic consists in expressing real-life industrial problems into these mathematical frameworks. Regarding statistical methods, the team works on dimension reduction models. They provide a way to understand and visualize the structure of complex data sets. Furthermore, they are important tools in several different areas such as data analysis and machine learning, and appear in many applications such as biology, genetics, environment and recommendation systems. Our contribution to this topic consists in studying semiparametric modeling which combines the advantages of parametric and nonparametric models.

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. 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 [40] and Duan and Li [38].
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 [39].

Stochastic control: optimal stopping, impulse control, continuous control, linear programming.
The main objective is to develop *approximation techniques* to provide quasi-optimal feasible solutions and to derive *optimality results* for control problems related to MDPs and PDMPs:

- *Approximation techniques*. The analysis and the resolution of such decision models mainly rely on the maximum principle and/or the dynamic/linear programming techniques together with their various extensions such as the value iteration (VIA) and the policy iteration (PIA) algorithm. However, it is well known that these approaches are hardly applicable in practice and suffer from the so-called *curse of dimensionality*. Hence, solving numerically a PDMP or an MDP is a difficult and important challenge. Our goal is to obtain results which are both consistent from a theoretical point of view and computationally tractable and accurate from an application standpoint. It is important to emphasize that these research objectives were not planned in our initial 2009 program.

  Our objective is to propose approximation techniques to efficiently compute the optimal value function and to get quasi-optimal controls for different classes of constrained and unconstrained MDPs with general state/action spaces, and possibly unbounded cost function. Our approach is based on combining the linear programming formulation of an MDP with probabilistic approximation techniques related to quantization techniques and the theory of empirical processes. An other aim is to apply our methods to specific industrial applications in collaboration with industrial partners such as Airbus Defence & Space, Naval Group and Thales.

  Asymptotic approximations are also developed in the context of queueing networks, a class of models where the decision policy of the underlying MDP is in some sense fixed a priori, and our main goal is to study the transient or stationary behavior of the induced Markov process. Even though the decision policy is fixed, these models usually remain intractable to solve. Given this complexity, the team has developed analyses in some limiting regime of practical interest, i.e., queueing models in the large-network, heavy-traffic, fluid or mean-field limit. This approach is helpful to obtain a simpler mathematical description of the system under investigation, which is often given in terms of ordinary differential equations or convex optimization problems.

- *Optimality results*. Our aim is to investigate new important classes of optimal stochastic control problems including constraints and combining continuous and impulse actions for MDPs and PDMPs. In this framework, our objective is to obtain different types of optimality results. For example, we intend to provide conditions to guarantee the existence and uniqueness of the optimality equation for the problem under consideration and to ensure existence of an optimal (and ϵ-optimal) control strategy. We also plan to analyze the structural properties of the optimal strategies as well as to study the associated infinite dimensional linear programming problem. These results can be seen as a first step toward the development of numerical approximation techniques in the sense described above.

MATHRISK Project-Team

3. Research Program

3.1. Risk management: modeling and optimization

3.1.1. Contagion modeling and systemic risk

After the recent financial crisis, systemic risk has emerged as one of the major research topics in mathematical finance. Interconnected systems are subject to contagion in time of distress. 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.

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. [40] and A. Minca [79]) or mean field interaction models (Garnier-Papanicolaou-Yang [70]).

We have contributed in the last years to the research on the control of contagion in financial systems in the framework of random graph models : In [41], [80], [5], A. Sulem with A. Minca and H. Amini consider a financial network described as a weighted directed graph, in which nodes represent financial institutions and edges the exposures between them. The distress propagation is modeled as an epidemics on this graph. They study the optimal intervention of a lender of last resort who seeks to make equity infusions in a banking system prone to insolvency and to bank runs, under complete and incomplete information of the failure cluster, in order to minimize the contagion effects. The paper [5] provides in particular important insight on the relation between the value of a financial system, connectivity and optimal intervention.

The results show that up to a certain connectivity, the value of the financial system increases with connectivity. However, this is no longer the case if connectivity becomes too large. The natural question remains how to create incentives for the banks to attain an optimal level of connectivity. This is studied in [54], where network formation for a large set of financial institutions represented as nodes is investigated. Linkages are source of income, and at the same time they bear the risk of contagion, which is endogeneous and depends on the strategies of all nodes in the system. The optimal connectivity of the nodes results from a game. Existence of an equilibrium in the system and stability properties is studied. The results suggest that financial stability is best described in terms of the mechanism of network formation than in terms of simple statistics of the network topology like the average connectivity.

3.1.2. Liquidity risk and Market Microstructure

Liquidity risk is the risk arising from the difficulty of selling (or buying) an asset. 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, but 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), it 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.

For rather liquid assets, liquidity risk is usually taken into account via price impact models which describe how a (large) trader influences the asset prices. Then, one is typically interested in the optimal execution problem: how to buy/sell a given amount of assets optimally within a given deadline. This issue is directly related to the existence of statistical arbitrage or Price Manipulation Strategies (PMS). Most of price impact models deal with single assets. A. Alfonsi, F. Klöck and A. Schied [39] have proposed a multi-assets price impact model that extends previous works. Price impact models are usually relevant when trading at an intermediary frequency (say every hour). At a lower frequency, price impact is usually ignored while at a high frequency (every minute or second), one has to take into account the other traders and the price jumps, tick by tick. Midpoint price models are thus usually preferred at this time scale. With P. Blanc, Alfonsi [3] has proposed a model that makes a bridge between these two types of model: they have considered an (Obizhaeva and Wang) price impact model, in which the flow of market orders generated by the other traders is given by an exogeneous process. They have shown that Price Manipulation Strategies exist when the flow of order is a compound Poisson process. However, modeling this flow by a mutually exciting Hawkes process with a particular parametrization allows them to exclude these PMS. Besides, the optimal execution strategy is explicit in this model. A practical implementation is given in [35].

3.1.3. Dependence modeling

- Calibration of stochastic and local volatility models. The volatility is a key concept in modern mathematical finance, and an indicator of market stability. Risk management and associated instruments depend strongly on the volatility, and volatility modeling is a crucial issue in the finance industry. Of particular importance is the assets *dependence* modeling.

By Gyongy's theorem, a local and stochastic volatility model is calibrated to the market prices of all call options with positive maturities and strikes if its local volatility function is equal to the ratio of the Dupire local volatility function over the root conditional mean square of the stochastic volatility factor given the spot value. This leads to a SDE nonlinear in the sense of McKean. Particle methods based on a kernel approximation of the conditional expectation, as presented by Guyon and Henry-Labordère [71], provide an efficient calibration procedure even if some calibration errors may appear when the range of the stochastic volatility factor is very large. But so far, no existence result is available for the SDE nonlinear in the sense of McKean. In the particular case when the local volatility function is equal to the inverse of the root conditional mean square of the stochastic volatility factor multiplied by the spot value given this value and the interest rate is zero, the solution to the SDE is a fake Brownian motion. When the stochastic volatility factor is a constant (over time) random variable taking finitely many values and the range of its square is not too large, B. Jourdain and A. Zhou proved existence to the associated Fokker-Planck equation [77]. Thanks to results obtained by Figalli in [63], they deduced existence of a new class of fake Brownian motions. They extended these results to the special case of the LSV model called Regime Switching Local Volatility, when the stochastic volatility factor is a jump process taking finitely many values and with jump intensities depending on the spot level.

- Interest rates modeling. Affine term structure models have been popularized by Dai and Singleton [55], Duffie, Filipovic and Schachermayer [56]. They consider vector affine diffusions (the coordinates are usually called factors) and assume that the short interest rate is a linear combination of these factors. A model of this kind is the Linear Gaussian Model (LGM) that considers a vector Ornstein-Uhlenbeck diffusions for the factors, see El Karoui and Lacoste [62]. A. Alfonsi et al. [33] have proposed an extension of this model, when the instantaneous covariation between the factors is given by a Wishart process. Doing so, the model keeps its affine structure and tractability while generating smiles for option prices. A price expansion around the LGM is obtained for Caplet and Swaption prices.

3.1.4. Robust finance

- Numerical Methods for Martingale Optimal Transport problems.

The Martingale Optimal Transport (MOT) problem introduced in [53] has received a recent attention in finance since it gives model-free hedges and bounds on the prices of exotic options. The market prices of liquid call and put options give the marginal distributions of the underlying asset at each traded maturity. Under the simplifying assumption that the risk-free rate is zero, these probability measures are in increasing convex

order, since by Strassen's theorem this property is equivalent to the existence of a martingale measure with the right marginal distributions. For an exotic payoff function of the values of the underlying on the time-grid given by these maturities, the model-free upper-bound (resp. lower-bound) for the price consistent with these marginal distributions is given by the following martingale optimal transport problem : maximize (resp. minimize) the integral of the payoff with respect to the martingale measure over all martingale measures with the right marginal distributions. Super-hedging (resp. sub-hedging) strategies are obtained by solving the dual problem. With J. Corbetta, A. Alfonsi and B. Jourdain [36] have studied sampling methods preserving the convex order for two probability measures μ and ν on $\mathbf{R}^d$, with ν dominating μ.

Their method is the first generic approach to tackle the martingale optimal transport problem numerically and can also be applied to several marginals.

- Robust option pricing in financial markets with imperfections.

A. Sulem, M.C. Quenez and R. Dumitrescu have studied robust pricing in an imperfect financial market with default. The market imperfections are taken into account via the nonlinearity of the wealth dynamics. In this setting, the pricing system is expressed as a nonlinear g-expectation $\mathcal{E}^g$ induced by a nonlinear BSDE with nonlinear driver g and default jump (see [24]). A large class of imperfect market models can fit in this framework, including imperfections coming from different borrowing and lending interest rates, taxes on profits from risky investments, or from the trading impact of a large investor seller on the market prices and the default probability. Pricing and superhedging issues for American and game options in this context and their links with optimal stopping problems and Dynkin games with nonlinear expectation have been studied. These issues have also been addressed in the case of model uncertainty, in particular uncertainty on the default probability. The seller's robust price of a game option has been characterized as the value function of a Dynkin game under $\mathcal{E}^g$ expectation as well as the solution of a nonlinear doubly reflected BSDE in [9]. Existence of robust superhedging strategies has been studied. The buyer's point of view and arbitrage issues have also been studied in this context.

In a Markovian framework, the results of the paper [8] on combined optimal stopping/stochastic control with $\mathcal{E}^g$ expectation allows us to address American nonlinear option pricing when the payoff function is only Borelian and when there is ambiguity both on the drift and the volatility of the underlying asset price process. Robust optimal stopping of dynamic risk measures induced by BSDEs with jumps with model ambiguity is studied in [82].

3.2. Perspectives in Stochastic Analysis

3.2.1. Optimal transport and longtime behavior of Markov processes

The dissipation of general convex entropies for continuous time Markov processes can be described in terms of backward martingales with respect to the tail filtration. The relative entropy is the expected value of a backward submartingale. In the case of (non necessarily reversible) Markov diffusion processes, J. Fontbona and B. Jourdain [65] used Girsanov theory to explicit the Doob-Meyer decomposition of this submartingale. They deduced a stochastic analogue of the well known entropy dissipation formula, which is valid for general convex entropies, including the total variation distance. Under additional regularity assumptions, and using Itô's calculus and ideas of Arnold, Carlen and Ju [42], they obtained a new Bakry-Emery criterion which ensures exponential convergence of the entropy to 0. This criterion is non-intrinsic since it depends on the square root of the diffusion matrix, and cannot be written only in terms of the diffusion matrix itself. They provided examples where the classic Bakry Emery criterion fails, but their non-intrinsic criterion applies without modifying the law of the diffusion process.

With J. Corbetta, A. Alfonsi and B. Jourdain have studied the time derivative of the Wasserstein distance between the marginals of two Markov processes. The Kantorovich duality leads to a natural candidate for this derivative. Up to the sign, it is the sum of the integrals with respect to each of the two marginals of the corresponding generator applied to the corresponding Kantorovich potential. For pure jump processes with bounded intensity of jumps, J. Corbetta, A. Alfonsi and B. Jourdain [15] proved that the evolution of the Wasserstein distance is actually given by this candidate. In dimension one, they showed that this remains

true for Piecewise Deterministic Markov Processes. They applied the formula to estimate the exponential decrease rate of the Wasserstein distance between the marginals of two birth and death processes with the same generator in terms of the Wasserstein curvature.

3.2.2. Mean-field systems: modeling and control

- Mean-field limits of systems of interacting particles. In [75], B. Jourdain and his former PhD student J. Reygner have studied a mean-field version of rank-based models of equity markets such as the Atlas model introduced by Fernholz in the framework of Stochastic Portfolio Theory. They obtained an asymptotic description of the market when the number of companies grows to infinity. Then, they discussed the long-term capital distribution, recovering the Pareto-like shape of capital distribution curves usually derived from empirical studies, and providing a new description of the phase transition phenomenon observed by Chatterjee and Pal. They have also studied multitype sticky particle systems which can be obtained as vanishing noise limits of multitype rank-based diffusions (see [74]). Under a uniform strict hyperbolicity assumption on the characteristic fields, they constructed a multitype version of the sticky particle dynamics. In [76], they obtain the optimal rate of convergence as the number of particles grows to infinity of the approximate solutions to the diagonal hyperbolic system based on multitype sticky particles and on easy to compute time discretizations of these dynamics.

In [69], N. Fournier and B. Jourdain are interested in the two-dimensional Keller-Segel partial differential equation. This equation is a model for chemotaxis (and for Newtonian gravitational interaction).

- Mean field control and Stochastic Differential Games (SDGs). To handle situations where controls are chosen by several agents who interact in various ways, one may use the theory of Stochastic Differential Games (SDGs). Forward–Backward SDG and stochastic control under Model Uncertainty are studied in [83] by A. Sulem and B. Øksendal. Also of interest are large population games, where each player interacts with the average effect of the others and individually has negligible effect on the overall population. Such an interaction pattern may be modeled by mean field coupling and this leads to the study of mean-field stochastic control and related SDGs. A. Sulem, Y. Hu and B. Øksendal have studied singular mean field control problems and singular mean field two-players stochastic differential games [72]. Both sufficient and necessary conditions for the optimal controls and for the Nash equilibrium are obtained. Under some assumptions, the optimality conditions for singular mean-field control are reduced to a reflected Skorohod problem. Applications to optimal irreversible investments under uncertainty have been investigated. Predictive mean-field equations as a model for prices influenced by beliefs about the future are studied in [85].

3.2.3. Stochastic control and optimal stopping (games) under nonlinear expectation

M.C. Quenez and A. Sulem have studied optimal stopping with nonlinear expectation $\mathcal{E}^g$ induced by a BSDE with jumps with nonlinear driver g and irregular obstacle/payoff (see [82]). In particular, they characterize the value function as the solution of a reflected BSDE. This property is used in [19] to address American option pricing in markets with imperfections. The Markovian case is treated in [59] when the payoff function is continuous.

In [8], M.C. Quenez, A. Sulem and R. Dumitrescu study a combined optimal control/stopping problem under nonlinear expectation $\mathcal{E}^g$ in a Markovian framework when the terminal reward function is only Borelian. In this case, the value function u associated with this problem is irregular in general. They establish a *weak* dynamic programming principle (DPP), from which they derive that the upper and lower semi-continuous envelopes of u are the sub- and super- *viscosity solution* of an associated nonlinear Hamilton-Jacobi-Bellman variational inequality.

The problem of a generalized Dynkin game problem with nonlinear expectation $\mathcal{E}^g$ is addressed in [60]. Under Mokobodzki's condition, we establish the existence of a value function for this game, and characterize this value as the solution of a doubly reflected BSDE. The results of this work are used in [9] to solve the problem of game option pricing in markets with imperfections.

A generalized mixed game problem when the players have two actions: continuous control and stopping is studied in a Markovian framework in [61]. In this work, dynamic programming principles (DPP) are established: a strong DPP is proved in the case of a regular obstacle and a weak one in the irregular case. Using these DPPs, links with parabolic partial integro-differential Hamilton-Jacobi- Bellman variational inequalities with two obstacles are obtained.

With B. Øksendal and C. Fontana, A. Sulem has contributed on the issues of robust utility maximization [84], [85], and relations between information and performance [64].

3.2.4. Generalized Malliavin calculus

Vlad Bally has extended the stochastic differential calculus built by P. Malliavin which allows one to obtain integration by parts and associated regularity probability laws. In collaboration with L. Caramellino (Tor Vegata University, Roma), V. Bally has developed an abstract version of Malliavin calculus based on a splitting method (see [44]). It concerns random variables with law locally lower bounded by the Lebesgue measure (the so-called Doeblin's condition). Such random variables may be represented as a sum of a "smooth" random variable plus a rest. Based on this smooth part, he achieves a stochastic calculus which is inspired from Malliavin calculus [6]. An interesting application of such a calculus is to prove convergence for irregular test functions (total variation distance and more generally, distribution distance) in some more or less classical frameworks as the Central Limit Theorem, local versions of the CLT and moreover, general stochastic polynomials [48]. An exciting application concerns the number of roots of trigonometric polynomials with random coefficients [49]. Using Kac Rice lemma in this framework one comes back to a multidimensional CLT and employs Edgeworth expansions of order three for irregular test functions in order to study the mean and the variance of the number of roots. Another application concerns U statistics associated to polynomial functions. The techniques of generalized Malliavin calculus developed in [44] are applied in for the approximation of Markov processes (see [52] and [51]). On the other hand, using the classical Malliavin calculus, V. Bally in collaboration with L. Caramellino and P. Pigato studied some subtle phenomena related to diffusion processes, as short time behavior and estimates of tubes probabilities (see [46], [47], [45]).

3.3. Numerical Probability

Our project team is very much involved in numerical probability, aiming at pushing numerical methods towards the effective implementation. This numerical orientation is supported by a mathematical expertise which permits a rigorous analysis of the algorithms and provides theoretical support for the study of rates of convergence and the introduction of new tools for the improvement of numerical methods. This activity in the MathRisk team is strongly related to the development of the Premia software.

3.3.1. Simulation of stochastic differential equations

3.3.1.1. - Weak convergence of the Euler scheme in optimal transport distances.

With A. Kohatsu-Higa, A. Alfonsi and B. Jourdain [4] have proved using optimal transport tools that the Wasserstein distance between the time marginals of an elliptic SDE and its Euler discretization with N steps is not larger than $C\sqrt{\log(N)}/N$. The logarithmic factor may is removed when the uniform time-grid is replaced by a grid still counting N points but refined near the origin of times.

3.3.1.2. - Strong convergence properties of the Ninomiya Victoir scheme and multilevel Monte-Carlo estimators.

With their former PhD student, A. Al Gerbi, E. Clément and B. Jourdain [1] have proved strong convergence with order $1/2$ of the Ninomiya-Victoir scheme which is known to exhibit order 2 of weak convergence [81]. This study was aimed at analysing the use of this scheme either at each level or only at the finest level of a multilevel Monte Carlo estimator : indeed, the variance of a multilevel Monte Carlo estimator is related to the strong error between the two schemes used in the coarse and fine grids at each level. In [14], they proved that the order of strong convergence of the crude Ninomiya Victoir scheme is improved to 1 when the vector fields corresponding to each Brownian coordinate in the SDE commute, and in [34], they studied the error introduced by discretizing the ordinary differential equations involved in the Ninomiya-Victoir scheme.

3.3.1.3. - Non-asymptotic error bounds for the multilevel Monte Carlo Euler method.

A. Kebaier and B. Jourdain are interested in deriving non-asymptotic error bounds for the multilevel Monte Carlo method. As a first step, they dealt in [73] with the explicit Euler discretization of stochastic differential equations with a constant diffusion coefficient. They obtained Gaussian-type concentration. To do so, they used the Clark-Ocone representation formula and derived bounds for the moment generating functions of the squared difference between a crude Euler scheme and a finer one and of the squared difference of their Malliavin derivatives. The estimation of such differences is much more complicated than the one of a single Euler scheme contribution and explains why they suppose the diffusion coefficient to be constant. This assumption ensures boundedness of the Malliavin derivatives of both the SDE and its Euler scheme.

3.3.1.4. - Computation of sensibilities of integrals with respect to the invariant measure.

In [43], R. Assaraf, B. Jourdain, T. Lelièvre and R. Roux considered the solution to a stochastic differential equation with constant diffusion coefficient and with a drift function which depends smoothly on some real parameter λ, and admitting a unique invariant measure for any value of λ around $\lambda = 0$. Their aim was to compute the derivative with respect to λ of averages with respect to the invariant measure, at $\lambda = 0$. They analyzed a numerical method which consists in simulating the process at $\lambda = 0$ together with its derivative with respect to λ on a long time horizon. They gave sufficient conditions implying uniform-in-time square integrability of this derivative. This allows in particular to compute efficiently the derivative with respect to λ of the mean of an observable through Monte Carlo simulations.

3.3.1.5. - Approximation of doubly reflected Backward stochastic differential equations.

R. Dumitrescu and C. Labart have studied the discrete time approximation scheme for the solution of a doubly reflected Backward Stochastic Differential Equation with jumps, driven by a Brownian motion and an independent compensated Poisson process [58], [57].

3.3.1.6. - Parametrix methods.

V. Bally and A. Kohatsu-Higa have recently proposed an unbiased estimator based on the parametrix method to compute expectations of functions of a given SDE ([50]). This method is very general, and A. Alfonsi, A. Kohastu-Higa and M. Hayashi [37] have applied it to the case of one-dimensional reflected diffusions. In this case, the estimator can be obtained explicitly by using the scheme of Lépingle [78] and is quite simple to implement. It is compared to other simulation methods for reflected SDEs.

3.3.2. Estimation of the parameters of a Wishart process

A. Alfonsi, A. Kebaier and C. Rey [38] have computed the Maximum Likelihood Estimator for the Wishart process and studied its convergence in the ergodic and in some non ergodic cases. In the ergodic case, which is the most relevant for applications, they obtain the standard square-root convergence. In the non ergodic case, the analysis rely on refined results for the Laplace transform of Wishart processes, which are of independent interest.

3.3.3. Optimal stopping and American options

In joint work with A. Bouselmi, D. Lamberton studied the asymptotic behavior of the exercise boundary near maturity for American put options in exponential Lévy models. In [7], they deal with jump-diffusion models, and establish that, in some cases, the behavior differs from the classical Black and Scholes setting. D. Lamberton has also worked on the binomial approximation of the American put. The conjectured rate of convergence is $O(1/n)$ where n is the number of time periods. He was able to derive a $O((\ln n)^{\alpha}/n)$ bound, where the exponent α is related to the asymptotic behavior of the exercise boundary near maturity.

SIMSMART Team

3. Research Program

3.1. Research Program

Introduction. Computer simulation of physical systems is becoming increasingly reliant on highly complex models, as the constant surge of computational power is nurturing scientists into simulating the most detailed features of reality – from complex molecular systems to climate/weather forecast.

Yet, when modeling physical reality, bottom-up approaches are stumbling over intrinsic difficulties. First, the timescale separation between the fastest simulated microscopic features, and the macroscopic effective slow behavior becomes huge, implying that the fully detailed and direct long time simulation of many interesting systems (*e.g.* large molecular systems) are out of reasonable computational reach. Second, the chaotic dynamical behaviors of the systems at stake, coupled with such multi-scale structures, exacerbate the intricate uncertainty of outcomes, which become highly dependent on intrinsic chaos, uncontrolled modeling, as well as numerical discretization. Finally, the massive increase of observational data addresses new challenges to classical data assimilation, such as dealing with high dimensional observations and/or extremely long time series of observations.

SIMSMART Identity. Within this highly challenging applicative context, SIMSMART positions itself as a computational probability and statistics research team, with a mathematical perspective. Our approach is based on the use of *stochastic modeling* of complex physical systems, and on the use of *Monte Carlo simulation* methods, with a strong emphasis on dynamical models. The two main numerical tasks of interest to SIMSMART are the following: (i) simulating with pseudo-random number generators - a.k.a. *sampling* - dynamical models of random physical systems, (ii) sampling such random physical dynamical models given some real observations - a.k.a. *Bayesian data assimilation*. SIMSMART aims at providing an appropriate mathematical level of abstraction and generalization to a wide variety of Monte Carlo simulation algorithms in order to propose non-superficial answers to both *methodological and mathematical* challenges. The issues to be resolved include computational complexity reduction, statistical variance reduction, and uncertainty quantification.

SIMSMART's Objectives. The main objective of SIMSMART is to disrupt this now classical field of particle Monte Carlo simulation by creating deeper mathematical frameworks adapted to the challenging world of complex (*e.g.* high dimensional and/or multi-scale), and massively observed systems, as described in the beginning of this introduction.

To be more specific, we will classify SIMSMART objectives using the following four intertwined topics:

1. Objective 1: Rare events and random simulation.
2. Objective 2: High dimensional and advanced particle filtering.
3. Objective 3: Non-parametric approaches.
4. Objective 4: Model reduction and sparsity.

Rare events Objective 1 are ubiquitous in random simulation, either to accelerate the occurrence of physically relevant random slow phenomenons, or to estimate the effect of uncertain variables. Objective 1 will be mainly concerned with particle methods where *splitting* is used to enforce the occurrence of rare events.

The problem of high dimensional observations, the main topic in Objective 2, is a known bottleneck in filtering, especially in non-linear particle filtering, where linear data assimilation methods remain the state-of-the-art approaches.

The increasing size of recorded observational data and the increasing complexity of models also suggest to devote more effort into non-parametric data assimilation methods, the main issue of Objective 3.

In some contexts, for instance when one wants to compare solutions of a complex (*e.g.* high dimensional) dynamical systems depending on uncertain parameters, the construction of relevant reduced-order models becomes a key topic. This is the content of Objective 4.

With respect to volume of research activity, Objective 1, Objective 4 and the sum (Objective 2+Objective 3) are comparable.

Some new challenges in the simulation and data assimilation of random physical dynamical systems have become prominent in the last decade. A first issue (i) consists in the intertwined problems of simulating on large, macroscopic random times, and simulating *rare events*. The link between both aspects stems from the fact that many effective, large times dynamics can be approximated by sequences of rare events. A second, obvious, issue (ii) consists in managing *very abundant observational data*. A third issue (iii) consists in quantifying *uncertainty/sensitivity/variance* of outcomes with respect to models or noise. A fourth issue (iv) consists in managing *high dimensionality*, either when dealing with complex prior physical models, or with very large data sets. The related increase of complexity also requires, as a fifth issue (v), the construction of *reduced models* to speed-up comparative simulations. In a context of very abundant data, this may be replaced by a sixth issue (vi) where complexity constraints on modeling is replaced by the use of *non-parametric statistical inference*.

Hindsight suggests that all the latter challenges are related. Indeed, the contemporary digital condition, made of a massive increase in computational power and in available data, is resulting in a demand for more complex and uncertain models, for more extreme regimes, and for using inductive approaches relying on abundant data.

For simplicity, we have classified SIMSMART research into the following already mentioned four main objectives.

1. Objective 1: Rare events and random simulation, which mainly encompass item (i).
2. Objective 2: High dimension and advanced particle filtering, which encompass item (iv).
3. Objective 3: Non-parametric inference, which mainly encompass item (ii) and (vi).
4. Objective 4: Model reduction, which mainly encompasses item (vi).

Uncertainty quantification (item (iii)) in fact underlies each aspect since we are mainly interested in Monte Carlo approaches, so that uncertainty can be *modeled by an initial random variable and be incorporated in the state space of the physical model*.

TOSCA Project-Team

3. Research Program

3.1. Research Program

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

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

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