RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

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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 [107], or to the dynamics of turbulent flows for which large scale / small scale vortical structures interfere [136].

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 [76] for an existence result and [61], [75] 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 [67], [95] for some applications in traffic flow modelling, and [86], [91], [93] 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 [61], [75].

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 [68], [78] for the derivation of Lighthill-Whitham-Richards [119], [135] traffic flow model from Follow-the-Leader and [87] for results on crowd motion models (see also [109]). 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 [79], and extensively used since then to prove convergence of approximate solutions and deduce existence results, see for example [88] 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 [50], [90]. We refer, for example, to the notion of solution for non-hyperbolic systems [97], 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 [90].

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 [72]), and proved to be successful for studying emerging self-organised flow patterns [71]. The theoretical measure framework proves to be also relevant in addressing micro-macro limiting procedures of mean field type [98], 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* [143], [144]. Indeed, as observed in [126], 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 [118]). 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 [57], [58], [80], [117], 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 [131], 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 [74] 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, [48]) 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 [45], sedimentation [52], supply chains [101], conveyor belts [102], biological applications like structured populations dynamics [125], or more general problems like gradient constrained equations [46]. Also, non-local in time terms arise in conservation laws with memory, starting from [73]. 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 [53], [60], [64], [99], [139]. 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 [53], [99] 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 [47] for scalar equations in one space dimension ($N = d = 1$), in [65] for scalar equations in several space dimensions ($N = 1$, $d \geq 1$) and in [41], [66], [70] for multi-dimensional systems of conservation laws. Besides, specific finite volume numerical methods have been developed recently in [41], [99] and [116].

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 [59]. In aerodynamics, inflow conditions like velocity modulus and direction, are subject to fluctuations [105], [124]. For some engineering problems, the geometry of the boundary can also be uncertain, due to structural deformation, mechanical wear or disregard of some details [82]. 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 [137], [142], 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 [138], [141], 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 [123]. 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 [105], [114], [120], [146] or an entropy closure method [77], or by discretizing the probability space and extending the numerical schemes to the stochastic components [40]. 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 [132], [142], [145].

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 [51]. Besides, we plan to extend previous works on sensitivity analysis [82], [121] 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 [54] (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 [142]. 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 [134] 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 [49], [100] for the backward time integration of the adjoint variables. The sensitivity equation method (SEM) offers a promising alternative [81], [110], 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 [82].
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) [136] , Detached-Eddy Simulation (DES) [140] or Organized-Eddy Simulation (OES) [55], 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 [112] 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 [83] [84]. 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 [85] 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 [129] 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 [148].

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 [92]. 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 [42] 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 high values of the Reynolds number is governed by a spectrum of time and space scales fluctuations closely connected with the turbulent nature of the flow. The term deterministic chaos employed by Frisch in his enlightening book [32] is certainly conveying most adequately the difficulty in analyzing and simulating this kind of flows. The broadness of the turbulence spectrum is directly controlled by the Reynolds number defined as the ratio between the inertial forces and the viscous forces. This number is not only useful to determine the transition from a laminar to a turbulent flow regime, it also indicates the range of scales of fluctuations that are present in the flow under consideration. Typically, for the velocity field and far from solid walls, the ratio between the largest scale (the integral length scale) to the smallest one (Kolmogorov scale) scales as $Re^{3/4}$ per dimension. In addition, for internal flows, the viscous effects near the solid walls yield a scaling proportional to Re per dimension. The smallest scales play a crucial role in the dynamics of the largest ones which implies that an accurate framework for the computation of turbulent flows must take into account all these scales. Thus, the usual practice to deal with turbulent flows is to choose between an a priori modeling (in most situations) or not (low Re number and rather simple configurations) before proceeding to the discretization step followed by the simulation runs themselves. If a modeling phase is on the agenda, then one has to choose again among the above mentioned variety of approaches. As it is illustrated in Fig. 1 , this can be achieved either by directly solving the Navier-Stokes equations (DNS) or by first applying a statistical averaging (RANS) or a spatial filtering operator to the Navier-Stokes equations (LES). The new terms brought about by the filtering operator have to be modeled. From a computational point of view, the RANS approach is the least demanding, which explains why historically it has been the workhorse in both the academic and the industrial sectors. It has permitted quite a substantial progress in the understanding of various phenomena such as turbulent combustion or heat transfer. Its inherent inability to provide a time-dependent information has led to promote in the last decade the recourse to either LES or DNS to supplement if not replace RANS. By simulating the large scale structures while modeling the smallest ones supposed to be more isotropic, LES proved to be quite a step through that permits to fully take advantage of the increasing power of computers to study complex flow configurations. At the same time, DNS was progressively applied to geometries of increasing complexity (channel flows with values of Re_τ multiplied by 10 during the last 15 years, jets, turbulent premixed flames, among many others), and proved to be a formidable tool that permits **(i)** to improve our knowledge on turbulent flows and **(ii)** to test (i.e., validate or invalidate) and improve the modeling hypotheses inherently associated to the RANS and LES approaches. From a numerical point of view, if the steady nature of the RANS equations allows to perform iterative convergence on finer and finer meshes, the high computational cost of LES or DNS makes necessary the use of highly accurate numerical schemes in order to optimize the use of computational resources. To the noticeable exception of the hybrid RANS-LES modeling, which is not yet accepted as a reliable tool for industrial design, as mentioned in the preamble of the Go4hybrid European program [0], once chosen, a single turbulence model will (try to) do the job for modeling the whole flow. Thus, depending on its intrinsic strengths and weaknesses, the accuracy will be a rather volatile quantity strongly dependent on the flow configuration. The turbulence modeling and industrial design communities waver between the desire to continue to rely on the RANS approach, which is unrivaled in terms of computational cost, but is still not able to accurately represent all the complex phenomena; and the temptation to switch to LES, which outperforms RANS in many situations but is prohibitively expensive in high-Reynolds number wall-bounded flows. In order to account for the deficiencies of both approaches and to combine them for significantly improving the overall quality of

[0] https://cordis.europa.eu/result/rcn/177053_en.html

the modeling, the hybrid RANS-LES approach has emerged during the last decade as a viable, intermediate way, and we are definitely inscribing our project in this innovative field of research, with an original approach though, connected with a time filtered hybrid RANS-LES and a systematic and progressive validation process against experimental data produced by the team.

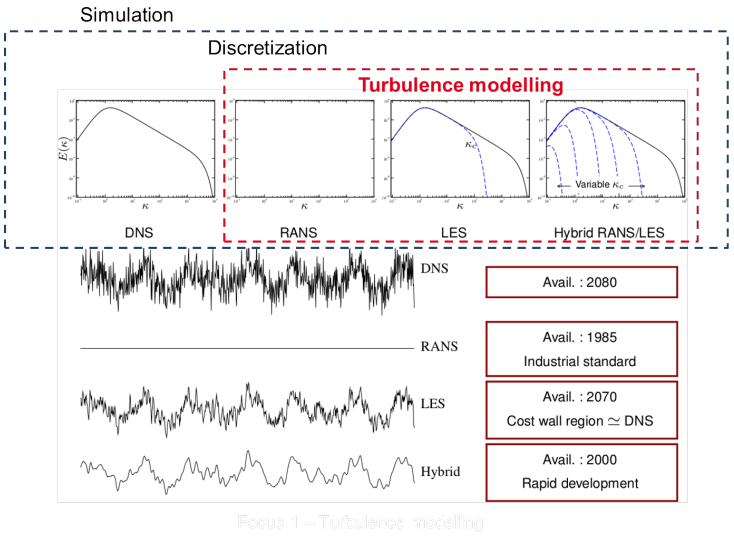

Figure 1. A schematic view of the different nested steps for turbulent flow simulation: from DNS to hybrid RANS-LES. The approximate dates at which the different approaches are or will be routinely used in the industry are indicated in the boxes on the right (extrapolations based on the present rate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

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

All the methods considered in the project are mesh-based methods: the computational domain is divided into cells, that have an elementary shape: triangles and quadrangles in two dimensions, and tetrahedra, hexahedra, pyramids, and prisms in three dimensions. If the cells are only regular hexahedra, the mesh is said to be structured. Otherwise, it is said to be unstructured. If the mesh is composed of more than one sort of elementary shape, the mesh is said to be hybrid. In the project, the numerical strategy is based on discontinuous Galerkin methods. These methods were introduced by Reed and Hill [43] and first studied by Lesaint and Raviart [39]. The extension to the Euler system with explicit time integration was mainly led by Shu, Cockburn and their collaborators. The steps of time integration and slope limiting were similar to high order ENO schemes, whereas specific constraints given by the finite element nature of the scheme were progressively solved, for scalar conservation laws [28], [27], one dimensional systems [26], multidimensional scalar conservation laws [25], and multidimensional systems [29]. For the same system, we can also cite the work of [31], [36], which is slightly different: the stabilization is made by adding a nonlinear term, and the time integration is implicit. Contrary to continuous Galerkin methods, the discretization of diffusive operators is not straightforward. This is due to the discontinuous approximation space, which does not fit well with the space function in which the diffusive system is well posed. A first stabilization was proposed by Arnold [18]. The first application of discontinuous Galerkin methods to Navier-Stokes equations was proposed in [23] by mean of a mixed formulation. Actually, this first attempt led to a non compact computation stencil, and was later proved to be not stable. A compactness improvement was made in [24], which was later analyzed, and proved to be stable

in a more unified framework [19]. The combination with the $k-\omega$ RANS model was made in [22]. As far as Navier Stokes equations are concerned, we can also cite the work of [34], in which the stabilization is closer to the one of [19], the work of [40] on local time stepping, or the first use of discontinuous Galerkin methods for direct numerical simulation of a turbulent channel flow done in [30]. Discontinuous Galerkin methods are so popular because:

- They can be developed for any order of approximation.
- The computational stencil of one given cell is limited to the cells with which it has a common face. This stencil does not depend on the order of approximation. This is a pro, compared for example with high order finite volumes, which require as more and more neighbors as the order increases.
- They can be developed for any kind of mesh, structured, unstructured, but also for aggregated grids [21]. This is a pro compared not only with finite differences schemes, which can be developed only on structured meshes, but also compared with continuous finite elements methods, for which the definition of the approximation basis is not clear on aggregated elements.
- p-adaptivity is easier than with continuous finite elements, because neighboring elements having a different order are only weakly coupled.
- Upwinding is as natural as for finite volumes methods, which is a benefit for hyperbolic problems.
- As the formulation is weak, boundary conditions are naturally weakly formulated. This is a benefit compared with strong formulations, for example point centered formulation when a point is at the intersection of two kinds of boundary conditions.

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

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

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

3.2. Research directions

3.2.1. Boundary conditions

3.2.1.1. Generating synthetic turbulence

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

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

3.2.1.2. Stable and non reflecting boundary conditions

In aerodynamics, and especially for subsonic computations, handling inlet and outlet boundary conditions is a difficult issue. A lot of work has already been done for second order schemes for Navier Stokes equations, see [42], [45] and the huge number of papers citing it. On the one hand, we believe that strong improvements are necessary with higher order schemes: indeed, the less dissipative the scheme is, the worse impact have the spurious reflections. For this, we will first concentrate on the linearized Navier-Stokes system, and analyze the boundary condition imposition in a discontinuous Galerkin framework with a similar approach as in [33]. We will also try to extend the work of [46], which deals with Euler equations, to the Navier Stokes equations.

3.2.2. Turbulence models and model agility

3.2.2.1. Extension of zero Mach models to the compressible system

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

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

In the targeted application domains, the turbulence/wall interaction and the heat transfer at the fluid-solid interfaces are physical phenomena whose numerical prediction is at the heart of the concerns of our industrial partners. For instance, for a jet engine manufacturer, being able to properly design the configuration of the cooling of the walls of its engine combustion chamber in the presence of thermoacoustic instabilities is based on the proper identification and a thorough understanding of the major mechanisms that drive the dynamics of the parietal transfers. For our part, we will gradually use all our analysis and experimentation tools to actively participate in the improvement of the collective knowledge on such kind of transfers. The flow configurations dealt with by the beginning of the project will be those of subsonic single phase impacting jets or JICF with the possible presence of an interacting acoustic wave. The conjugate heat transfer at the wall will be also progressively tackled. The existing criteria of switching of the hybrid RANS/LES model will be tested on those flow configurations in order to determine their domain of validity. In parallel, the hydrodynamic instability modes of the JICF will be studied experimentally and theoretically (in cooperation with the SIAME laboratory) in order to determine if it is possible to drive a change of instability regime (e.g. from absolute to convective) and so propose challenging flow conditions that would be relevant for the setting-up of an hybrid LES/DNS approach aimed at supplementing the hybrid RANS/LES one.

3.2.2.3. Improvement of turbulence models

The production and the subsequent use of DNS (AeroSol library) and experimental (bench MAVERIC) databases dedicated to the improvement of the physical models will be an important part of our activity. In that respect, our present capability of producing in-situ experimental data for simulation validation and flow analysis is clearly a strongly differentiating mark of our project. It is on the improvement of the hybrid RANS/LES approach that will focus most of our initial efforts of analysis of the DNS and experimental data as soon as they will become available. This method has a decisive advantage over all other hybrid

RANS/LES approaches since it relies on a well defined time filtering formalism. This greatly facilitates the proper extraction from the databases of the various terms appearing in the relevant flux balances obtained at the different scales involved (e.g. from RANS to LES). But we would not be comprehensive in that matter if we were not questioning the relevance of any simulation-experiment comparisons. In other words, a central issue will also be to answer positively the following question: will we be comparing the same quantities between simulations and experiment? From an experimental point of view, the questions to be raised will be, among others, the possible difference in resolution between the experiment and the simulations, the similar location of the measurement points and simulation points, the acceptable level of random error associated to the necessary finite number of samples. In that respect, the recourse to uncertainty quantification techniques will be advantageously considered.

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

As the flows we wish to simulate may be very computationally demanding, we will maintain our efforts in the development of AeroSol in the following directions:

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

3.2.3.1. Efficient implementation of the discontinuous Galerkin method

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

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

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

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

Using implicit time stepping in compressible flows in particularly difficult, because the system is fully nonlinear, so that the nonlinear solving theoretically requires to build many times the Jacobian. Our experience in implicit methods is that the building of a Jacobian is very costly, especially in three dimensions and in a high order framework, because the optimization of the memory usage is very difficult. That is why we propose to use Jacobian free implementation, based on [38]. 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 [47], [48] with the number of unknowns in term of number of operations, and that this preconditioning does not require any Jacobian computation.

Beyond the technical aspects of the multigrid approach, which will be challenging to implement, we are also interested in the design of an efficient aggregation. This often means to perform an aggregation based on criteria (anisotropy of the problem, for example) [41]. For this, we propose to extend the scalar analysis of [49] 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 [21].

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 [44]. Already in 2003, [35] pointed out the difficulties for efficiently using the biggest clusters: "While these super-clusters have theoretical peak performance applications is far from the peak. Salinas, one of the 2002 Gordon Bell Awards was able to sustain 1.16 Tflops on ASCI White (less than 10% of peak)." From the current multi-core architectures, the trend is now to use many-core accelerators. The idea behind many-core is to use an accelerator composed of a lot of relatively slow and simplified cores for executing the most simple parts of the algorithm. The larger the part of the code executed on the accelerator, the faster the code may become. In this task, we will work on the heterogeneous aspects of computation. These heterogeneities are intrinsic to our computations and have two sources. The first one is the use of hybrid meshes, which are necessary for using a local structured mesh in a boundary layer. As the different cell shapes (pyramids, hexahedra, prisms and tetrahedra) do not have the same number of degrees of freedom, nor the same number of quadrature points, the execution time on one face or one cell depends on its shape. The second source of heterogeneity are the boundary conditions. Depending on the kind of boundary conditions, user defined boundary values might be needed, which induces a different computational cost. Heterogeneities are typically what may decrease efficiency in parallel if the workload is not well balanced between the cores. Note that heterogeneities were not dealt with in what we consider as one of the most advanced work on discontinuous Galerkin on GPU [37], 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 [20]. For this, the discontinuous Galerkin algorithm will be reformulated in term of a graph of tasks. The previous tasks on the memory management will be useful for that. The linear steps of the discontinuous Galerkin methods require also memory transfers, and one task of the project will consist in determining the optimal task granularity for this step, i.e. the number of cells or face integrations to be sent in parallel on the accelerator. On top of that, the question of which device is the most appropriate to tackle such kind of tasks will be discussed.

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

The consortium will benefit from a particularly stimulating environment in the Inria Bordeaux Sud Ouest center around high performance computing, which is one of the strategic axis of the center.

3.2.3.4. Implementation of turbulence models in AeroSol and validation

We will gradually insert models developed in research direction 3.2.2.1 in the AeroSol library in which we develop methods for the DNS of compressible turbulent flows at low Mach number. Indeed, thanks to its formalism of temporal filtering, the HTLES approach offers a theoretical framework characterized by a

continuous transition from RANS to DNS, even for complex flow configurations (e.g. without directions of spatial homogeneity). As for the discontinuous Galerkin method available presently in AeroSol, it is the best suited and versatile method able to meet the requirements of accuracy, stability and cost related to the local (varying) level of resolution of the turbulent flow at hand, regardless of its configuration complexity. 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 [108], [112] 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 [57] to hybrid meshes (prism/tetra).

For time dependent adaptation we will try to exploit as much as possible the use of $r-$adaptation techniques based on the solution of some PDE system for the mesh. We will work on enhancing the initial results of [61], [63] by developing more robust nonlinear variants allowing to embed rapidly moving objects. For this the use of non-linear mesh PDEs (cf e.g. [122], [134], [75]), combined with Bezier type approximations for the mesh displacements to accommodate high order curved meshes [57], 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 [110], [115], [114] 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. [87], [141], [139] 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. [58], [97], [142], [84] and references therein).
The development of high order schemes for the discretization of the PDE will be a major part of our activity. We will work from the start in an Arbitrary Lagrangian Eulerian setting, so that mesh movement will be easily accommodated, and investigate the following main points:

- the ALE formulation is well adapted both to handle moving meshes, and to provide conservative, high order, and monotone remaps between different meshes. We want to address the issue of cost-accuracy of adaptive mesh computations by exploring different degrees of coupling between the flow and the mesh PDEs. Initial experience has indicated that a clever coupling may lead to a considerable CPU time reduction for a given resolution [63], [61]. 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 [62]. 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. [107]). The use of penalization will also provide a natural setting to compute immediate approximations of the forces on the immersed body [113], [116]. 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 [98], or on some iterative Defect Correction method (see e.g. [77]) ;

- 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 [93] 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 [124], [60], [125] 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 [76], allowing to have a more flexible approach similar to the so-called P^nP^m method [90], [130]. 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 [95] ;
- 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 [73], as well as spatial partitioning techniques [104]. 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 [56]. 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 [56], 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 [56] 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 [81] ;
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 in connection with wave imaging, structural design, non-destructive testing and medical imaging modalities. We are particularly interested in the development of fast methods that are suited for real-time applications and/or large scale problems. These goals require to work on both the physical and the mathematical models involved and indeed a solid expertise in related numerical algorithms.

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

By “imaging” we 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.

ECUADOR Project-Team

3. Research Program

3.1. Algorithmic Differentiation

Participants: Laurent Hascoët, Valérie Pascual, Ala Taftaf.

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

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

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

Algorithmic Differentiation (AD) differentiates *programs*. The input of AD is a source program P that, given some $X \in \mathbb{R}^n$, returns some $Y = F(X) \in \mathbb{R}^m$, for a differentiable F. AD generates a new source program P' that, given X, computes some derivatives of F [4].

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.

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 [30], adjoint problems [24], or inverse problems.

Adjoint AD builds a very efficient program [26], which computes the gradient in a time independent from the number of parameters n. In contrast, computing the same gradient with the *tangent mode* would require running the tangent differentiated program n times.

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

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

3.2. Static Analysis and Transformation of programs

Participants: Laurent Hascoët, Valérie Pascual, Ala Taftaf, Benoit Dufumier.

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 [17] 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 [20], [27], [18]. 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* [21] 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 [33], [22] 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 input parameters. Consider one particular scalar characteristic. Its sensitivity, (or gradient) with respect to the input parameters can be defined as the solution of "adjoint" equations, deduced from the original equations through linearization and transposition. The solution of the adjoint equations is known as the adjoint state.

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

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

- One can write an *adjoint system* of mathematical equations, then discretize it and program it by hand. This is time consuming. Although this looks mathematically sound [24], 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 [23] 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 [28], [31] 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 [25], [19] that combine low storage consumption with possible automated adjoint generation. We advocate incorporating them into the AD model and into the AD tools.

GAMMA3 Project-Team (section vide)

IPSO Project-Team

3. Research Program

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

Participants: Francois Castella, Philippe Chartier, Erwan Faou.

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

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

$$\begin{aligned} y'(t) &= f(y(t)), \\ y(0) &= y_0. \end{aligned} \tag{6}$$

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

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

3.1.1. Reversible ODEs

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

$$\rho \circ \varphi_t = \varphi_t^{-1} \circ \rho = \varphi_{-t} \circ \rho. \tag{7}$$

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

3.1.2. ODEs with an invariant manifold

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

$$\mathcal{M} = \{y \in \mathbb{R}^n; g(y) = 0\} \tag{8}$$

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

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

As an example, we mention Lie-group equations, for which the manifold has an additional group structure. This could possibly be exploited for the space-discretisation. Numerical methods amenable to this sort of problems have been reviewed in a recent paper [37] and divided into two classes, according to whether they use g explicitly or through a projection step. In both cases, the numerical solution is forced to live on the manifold at the expense of some Newton's iterations.

3.1.3. Hamiltonian systems

Hamiltonian problems are ordinary differential equations of the form:

$$\begin{array}{rcccl} \dot{p}(t) & = & -\nabla_q H(p(t),q(t)) & \in & \mathbb{R}^d \\ \dot{q}(t) & = & \nabla_p H(p(t),q(t)) & \in & \mathbb{R}^d \end{array} \tag{9}$$

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

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

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

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

where J is the *canonical symplectic* matrix

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

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

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

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

3.1.4. Differential-algebraic equations

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

$$\begin{array}{rcl} \dot{y}(t) & = & f(y(t),z(t)), \\ 0 & = & g(y(t)), \end{array} \tag{10}$$

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

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

and of the so-called hidden manifold

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

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

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

3.2. Highly-oscillatory systems

Participants: Francois Castella, Philippe Chartier, Nicolas Crouseilles, Erwan Faou, Florian Mehats, Mohammed Lemou.

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

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

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

$$\ddot{q} \quad = \quad -\nabla V(q) \tag{11}$$

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

$$h\omega < C,$$

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

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

$$i\dot{\psi}(t) = \frac{1}{\varepsilon} H(t)\psi(t), \tag{12}$$

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

3.3. Geometric schemes for the Schrödinger equation

Participants: Francois Castella, Philippe Chartier, Erwan Faou, Florian Mehats.

Schrödinger equation, variational splitting, energy conservation.

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

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

$$i\varepsilon \frac{\partial \psi}{\partial t} = H\psi, \tag{13}$$

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

$$H = T + V$$

with the kinetic and potential energy operators

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

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

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

The numerical approximation of (8) can be obtained using projections onto submanifolds of the phase space, leading to various PDEs or ODEs: see [41], [40] for reviews. However the long-time behavior of these approximated solutions is well understood only in this latter case, where the dynamics turns out to be finite dimensional. In the general case, it is very difficult to prove the preservation of qualitative properties of (8) such as energy conservation or growth in time of Sobolev norms. The reason for this is that backward error analysis is not directly applicable for PDEs. Overwhelming these difficulties is thus a very interesting challenge.

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

$$\psi_1 = \exp\left(-i(\delta t)V/2\right) \exp\left(i(\delta t)\Delta\right) \exp\left(-i(\delta t)V/2\right)\psi_0 \tag{14}$$

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

3.4. High-frequency limit of the Helmholtz equation

Participant: Francois Castella.

waves, Helmholtz equation, high oscillations.

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

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

$$i\alpha_\varepsilon u_\varepsilon(x) + \varepsilon^2 \Delta_x u_\varepsilon + n^2(x) u_\varepsilon = f_\varepsilon(x). \tag{15}$$

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

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

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

3.5. From the Schrödinger equation to Boltzmann-like equations

Participant: Francois Castella.

Schrödinger equation, asymptotic model, Boltzmann equation.

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

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

$$i\partial_t \psi(t,x) = -\frac{1}{2}\Delta_x \psi + V(x)\psi, \tag{16}$$

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

$$\partial_t f(t,x,v) = \int_{\mathbf{R}^3} \sigma(v,v') \, [f(t,x,v') - f(t,x,v)] dv'. \tag{17}$$

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

MATHERIALS Project-Team

3. Research Program

3.1. Research Program

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

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

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

MEMPHIS Project-Team

3. Research Program

3.1. Hierarchical Cartesian schemes

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

The approach that we plan to develop combines accurate enforcement of unfitted boundary conditions with adaptive octree and overset grids. The core idea is to use an octree/overset mesh for the approximation of the solution fields, while the geometry is captured by level set functions [37], [31] and boundary conditions are imposed using appropriate interpolation methods [22], [39], [35]. This eliminates the need for boundary conforming meshes that require time-consuming and error-prone mesh generation procedures, and opens the door for simulation of very complex geometries. In particular, it will be possible to easily import the industrial geometry and to build the associated level set function used for simulation.

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

3.2. Reduced-order models

Massive parallelization and rethinking of numerical schemes will allow the solution of new problem in physics and the prediction of new phenomena thanks to simulation. However, in industrial applications fast on line responses are needed for design and control. For instance, in the design process of an aircraft, the flight conditions and manoeuvres, which provide the largest aircraft loads, are not known a priori. Therefore the aerodynamic and inertial forces are calculated at a large number of conditions to give an estimate of the maximum loads, and hence stresses, that the structure of the detailed aircraft design will experience in service. A simplistic estimate of the number of analyses required would multiply the numbers of conditions to give 10^7. Even with simplistic models of the aircraft behavior this is an unfeasible number of separate simulations. However, engineering experience is used to identify the most likely critical loads conditions, meaning that approximately 10^5 simulations are required for conventional aircraft configurations. Furthermore these analyses have to be repeated every time that there is an update in the aircraft structure...

Compared to existing approaches for ROMs [28], our interest will be focused on two axis. On the one hand, we start from the consideration that small, highly non-linear scales are typically concentrated in limited spatial regions of the full simulation domain. So for example, in the flow past a wing, the highly non-linear phenomena take place close to the walls at the scale of a millimeter for computational domains that are of the order of hundreds of meters. In this context our approach is characterized by a multi-scale model where the large scales are described by far field models based on ROMs and the small scales are simulated by high-fidelity models. The whole point for this approach is to optimally decouple the far field from the near field.

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

However, thanks to Proper Orthogonal Decomposition (POD) [32], [38], [25] we can accurately approximate large solution databases using a small base. Recent techniques to investigate the temporal evolution of the POD modes (Koopman modes [33], [23], Dynamic Mode Decomposition [36]) allow a dynamic discrimination of the role played by each of them. This in turn can be exploited to interpolate between the modes in parameter space, thanks to ideas relying on optimal transportation [40], [27] that we have started developing in the FP7 project FFAST and H2020 AEROGUST. In the following we precise these ideas on a specific example.

MEPHYSTO Project-Team

3. Research Program

3.1. From statistical physics to continuum mechanics

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

At the continuum level, rubber is modelled by an energy E defined as the integral over a domain D of $\mathbb{R}^d$ of some energy density W depending only locally on the gradient of the deformation u: $E(u) = \int_D W(\nabla u(x))dx$. At the microscopic level (say 100nm), rubber is a network of cross-linked and entangled polymer chains (each chain is made of a sequence of monomers). At this scale the physics of polymer chains is well-understood in terms of statistical mechanics: monomers thermally fluctuate according to the Boltzmann distribution [42]. The associated Hamiltonian of a network is typically given by a contribution of the polymer chains (using self-avoiding random bridges) and a contribution due to steric effects (rubber is packed and monomers are surrounded by an excluded volume). The main challenge is to understand how this statistical physics picture yields rubber elasticity. Treloar assumed in [54] that for a piece of rubber undergoing some macroscopic deformation, the cross-links do not fluctuate and follow the macroscopic deformation, whereas between two cross-links, the chains fluctuate. This is the so-called affine assumption. Treloar's model is in rather good agreement with mechanical experiments in small deformation. In large deformation however, it overestimates the stress. A natural possibility to relax Treloar's model consists in relaxing the affine assumption while keeping the network description, which allows one to distinguish between different rubbers. This can be done by assuming that the deformation of the cross-links minimizes the free energy of the polymer chains, the deformation being fixed at the boundary of the macroscopic domain D. This gives rise to a "variational model". The analysis of the asymptotic behavior of this model as the typical length of a polymer chain vanishes has the same flavor as the homogenization theory of integral functionals in nonlinear elasticity (see [37], [48] in the periodic setting, and [39] in the random setting).

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

In collaboration with R. Alicandro (Univ. Cassino, Italy) and M. Cicalese (Univ. Munich, Germany), A. Gloria analyzed in [1] the (asymptotic) Γ-convergence of the variational model for rubber, in the case when the polymer chain network is represented by some ergodic random graph. The easiest such graph is the Delaunay tessellation of a point set generated as follows: random hard spheres of some given radius ρ are picked randomly until the domain is jammed (the so-called random parking measure of intensity ρ). With M. Penrose (Univ. Bath, UK), A. Gloria studied this random graph in this framework [5]. With P. Le Tallec (Mechanics department, Ecole polytechnique, France), M. Vidrascu (project-team REO, Inria Paris-Rocquencourt), and A. Gloria introduced and tested in [44] a numerical algorithm to approximate the homogenized energy density, and observed that this model compares well to rubber elasticity qualitatively.

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

3.2. Quantitative stochastic homogenization

Whereas the approximation of homogenized coefficients is an easy task in periodic homogenization, this is a highly nontrivial task for stochastic coefficients. This is in order to analyze numerical approximation methods of the homogenized coefficients that F. Otto (MPI for mathematics in the sciences, Leipzig, Germany) and A. Gloria obtained the first quantitative results in stochastic homogenization [3]. The development of a complete stochastic homogenization theory seems to be ripe for the analysis and constitutes the second major objective of this section.

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

$$\langle|\phi_\xi|^q\rangle < \infty \text{ for all } q \geq 1. \tag{18}$$

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

The proof of these results, which is inspired by [49], is based on the insight that coefficients such as the Poisson random inclusions are special in the sense that the associated probability measure satisfies a spectral gap estimate. Combined with elliptic regularity theory, this spectral gap estimate quantifies ergodicity in stochastic homogenization. This systematic use of tools from statistical physics has opened the way to the quantitative study of stochastic homogenization problems, which we plan to fully develop.

3.3. Nonlinear Schrödinger equations

As well known, the (non)linear Schrödinger equation

$$\partial_t\varphi(t,x) = -\Delta\varphi(t,x) + \lambda V(x)\varphi(t,x) + g|\varphi|^2\varphi(t,x), \quad \varphi(0,x) = \varphi_0(x) \tag{19}$$

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

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

$$i\partial_z\varphi(t,z) = -\beta(z)\partial_t^2\varphi(t,z) + \gamma(z)|\varphi(t,z)|^2\varphi(z,t), \tag{20}$$

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

If $g = 0, \lambda \neq 0$, V is a random potential, and φ_0 is deterministic, this is the standard random Schrödinger equation describing for example the motion of an electron in a random medium. The main issue in this setting is the determination of the regime of Anderson localization, a property characterized by the boundedness in time of the second moment $\int x^2 |\varphi(t,x)|^2 dx$ of the solution. If this second moment remains bounded in time, the solution is said to be localized. Whereas it is known that the solution is localized in one dimension for all (suitable) initial data, both localized and delocalized solutions exist in dimension 3 and it remains a major open problem today to prove this, cf. [41].

If now $g \neq 0, \lambda \neq 0$ and V is still random, but $|g| \ll \lambda$, a natural question is whether, and in which regime, one-dimensional Anderson localization perdures. Indeed, Anderson localization can be affected by the presence of the nonlinearity, which corresponds to an interaction between the electrons or atoms. Much numerical and some analytical work has been done on this issue (see for example [43] for a recent work at PhLAM, Laser physics department, Univ. Lille 1), but many questions remain, notably on the dependence of the result on the initial conditions, which, in a nonlinear system, may be very complex. The cold atoms team of PhLAM (Garreau-Szriftgiser) is currently setting up an experiment to analyze the effect of the interactions in a Bose-Einstein condensate on a closely related localization phenomenon called "dynamical localization", in the kicked rotor, see below.

3.4. Processes in random environment

In the course of developing a quantitative theory of stochastic homogenization of discrete elliptic equations, we have introduced new tools to quantify ergodicity in partial differential equations. These tools are however not limited to PDEs, and could also have an impact in other fields where an evolution takes place in a (possibly dynamic) random environment and an averaging process occurs. The goal is then to understand the asymptotics of the motion of the particle/process.

For a random walker in a random environment, the Kipnis-Varadhan theorem ensures that the expected squared-position of the random walker after time t is of order t (the prefactor depends on the homogenized coefficients). If instead of a random walk among random conductances we consider a particle with some initial velocity evolving in a random *potential* field according to the Newton law, the averaged squared-position at time t is expected to follow the scaling law t^2, see [34]. This is called stochastic acceleration.

Similar questions arise when the medium is reactive (that is, when the potential is modified by the particle itself). The approach to equilibrium in such systems was observed numerically and explained theoretically, but not completely proven, in [40].

Another related and more general direction of research is the validity of *universality principle* of statistical physics, which states that the qualitative behavior of physical systems depend on the microscopic details of the system only through some large-scale variables (the thermodynamic variables). Therefore, it is a natural problem in the field of interacting particle systems to obtain the macroscopic laws of the relevant thermodynamical quantities, using an underlying microscopic dynamics, namely particles that move according to some prescribed stochastic law. Probabilistically speaking, these systems are continuous time Markov processes.

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 [161] reformulated the problem as a variational problem subject to a convexity constraint. For more general models, and using ideas from Optimal Transportation, Carlier [89] considered the more general c-convexity constraint and proved a general existence result. Using the formulation of [89] McCann, Figalli and Kim [116] gave conditions under which the principal agent problem can be written as an infinite dimensional convex variational problem. The important results of [116] 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], [149], [146].
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 [92] 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], [121] 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], [59], [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 [90] used an Optimal Transportation approach to extend quantile regression to several dimensions. In this approach again, not only fixed marginals constraints are present but also constraints on conditional means. As in the martingale Optimal Transportation problem, one has to deal with an extra conditional constraint. The usual duality approach usually breaks down under such constraints and characterization of optimal couplings is a challenging task both from a theoretical and numerical viewpoint.

3.1.1.3. JKO gradient flows.

(*Participants:* G. Carlier, J-D. Benamou, M. Laborde, Q. Mérigot, V. Duval) The connection between the static and dynamic transportation problems (see Section 2.3) opens the door to many extensions, most notably by leveraging the use of gradient flows in metric spaces. The flow with respect to the transportation distance has been introduced by Jordan-Kindelherer-Otto (JKO) [129] 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 [129]), the porous medium equations, the granular media equation, just to give a few examples. It also finds application in image processing [78]. 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 [98])
- 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 [65]
- 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.

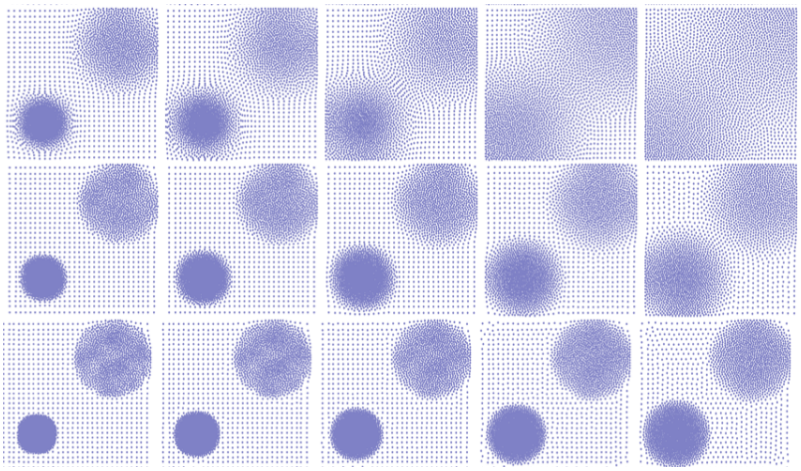

Figure 4. Example of non-linear diffusion equations solved with a JKO flow [55]. The horizontal axis shows the time evolution minimizing the functional $\int \frac{\rho^\alpha}{\alpha-1}$ on the density ρ (discretized here using point clouds, i.e. sum of Diracs' with equal mass). Each row shows a different 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 [59].
Goals: The case of general networks/anisotropies is still not well understood, general Γ-convergence results will be investigated as well as a detailed analysis of the corresponding PDEs and numerical methods to solve them. Benamou and Carlier already studied numerically some of these PDEs by an augmented Lagrangian method see figure 5 . Note that these class of problems share important similarities with metric learning problem in machine learning, detailed in Section 4.2 .

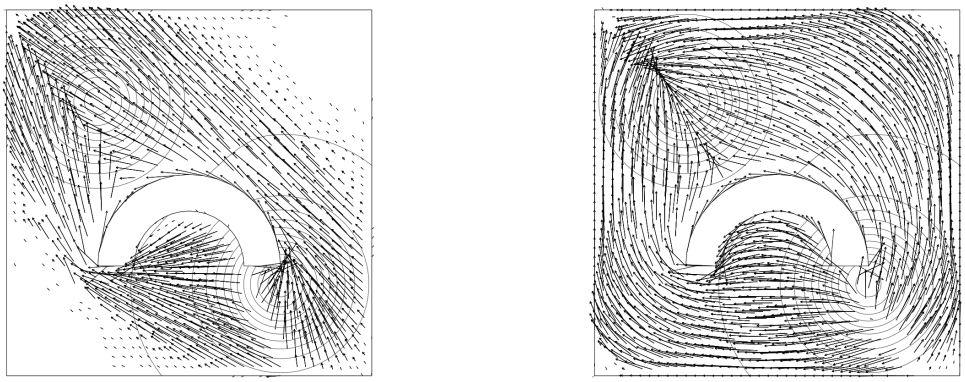

Figure 5. Monge and Wardrop flows of mass around an obstacle [52]. the source/target mass is represented by the level curves. Left : no congestion, Right : congestion.

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 [81] or tracking elastic organ movements [167]. Previous attempts [140], [157] 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 [133] with an extremely wide range of potential applications [124]. 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 [88] 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 [40].

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 [144] 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 [40], [77].
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) [173], [76], [171]. Our team has already studied flows and geodesics over non-Riemannian shape spaces, which allows for piecewise smooth deformations [102].

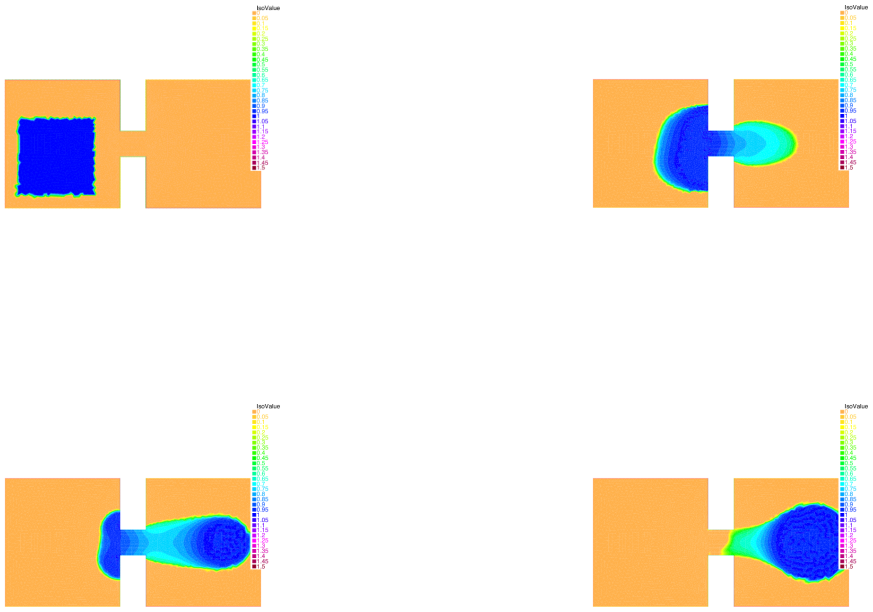

Figure 6. Example of crowd congestion with density dependent speed. The macroscopic density, at 4 different times, of people forced to exit from one room towards a meeting point in a second room.

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 [166], [167] 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 [135], 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 [174] 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 [117]. 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 [117], [118].
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 [172] 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 [66]) for discrete (finite dimensional) problems. We extended this result in a simple infinite dimensional setting, namely sparse regularization of Radon measures for deconvolution [112]. A deep understanding of those continuous inverse problems is crucial to analyze the behavior of their discrete counterparts, and in [113] 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

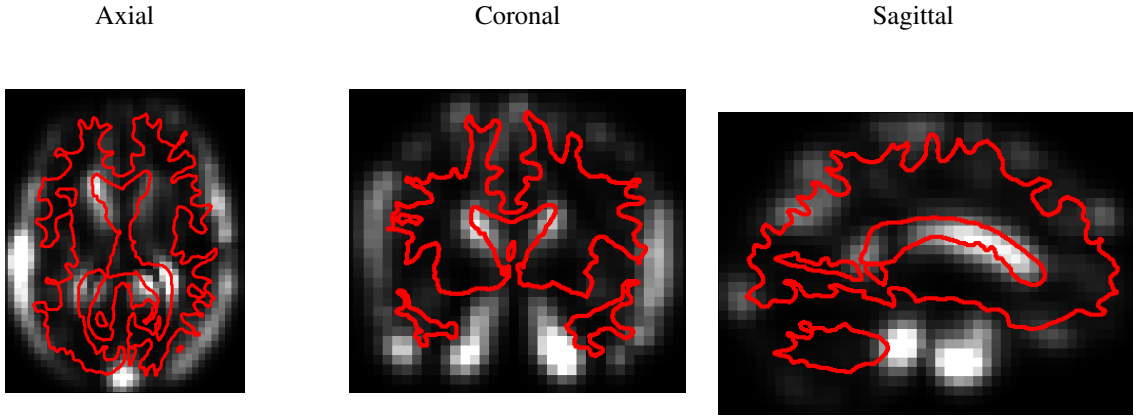

Figure 7. Learning Riemannian metrics in diffeomorphic image matching to capture the brain variability: a diagonal operator that encodes the Riemannian metric is learnt on a template brain out of a collection of brain images. The values of the diagonal operator are shown in greyscale. The red curves represent the boundary between white and grey matter. For more details, we refer the reader to [174], which was a first step towards designing effective and robust metric learning algorithms.

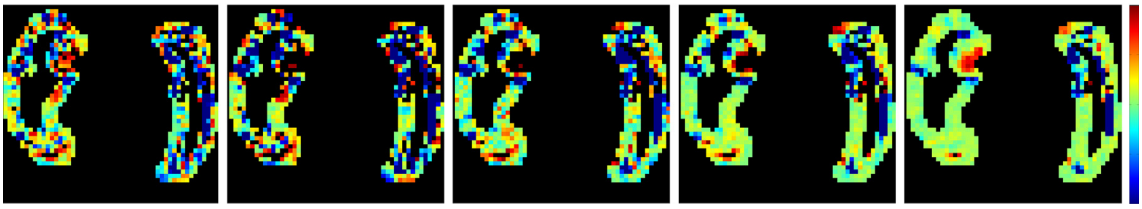

Figure 8. Statistics on initial momenta: In [117], we compared several intersubject transport methodologies to perform statistics on longitudinal evolutions. These longitudinal evolutions are represented by an initial velocity field on the shapes boundaries and these velocity fields are then compared 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 [91], [66] 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], [42], [99]. 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 [112] 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 [156], [114]. This requirement is also at the heart of recently proposed models of cortical processing [155]. 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 [147], [114]. G. Peyré has done several contributions on the definition of geometric wavelets transform and directional texture models, see for instance [156]. Dario Prandi has recently applied methods from sub-Riemannian geometry to image restoration [68].
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 [60]) 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 [126]. 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 [165]. Typical approaches [132] try to recovered piecewise smooth solutions in order to recover precisely the position of the organ being imaged. There is however a very poor understanding of the actual performance of these methods, and little is known on how to enhance the recovery.
Our expertise: We have obtained a good understanding of the performance of inverse problem regularization on *compact* domains for pointwise sources localization [112].
Goals: We aim at extending the theoretical performance analysis obtained for sparse measures [112] to the set of piecewise regular 2-D and 3-D functions. Some interesting previous work of C. Poon et al [158] (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 [39].

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 [81], [154] 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 [142], which are connected to so-called metamorphoses models in the LDDMM framework [61].
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 [81], [154] 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 [58] for the Monge-Ampère equation and [146] for general non-linear variational problems. Both offer convergence guarantees and are amenable to fast numerical resolution techniques such as Newton solvers. Since [58] 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 [120], a new different and more accurate approach has been proposed by Mirebeau, Benamou and Collino [56]. 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 [149] and J-M. Mirebeau [146]. 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 [129]) 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 [55] 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 [112], [113] 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 [112], [113] 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 [112] to generic partly-smooth convex regularizers routinely used in imaging science and machine learning, a prototypal example being the nuclear norm (see [172] 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], [112]. 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 [112] 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 [134]. 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 [163]), 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], [150], congested optimal transport [80] and to sparse regularizations (see for instance [160] 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 [150]. We have also recently developed new proximal schemes that can cope with non-smooth composite objectives functions [160].
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.

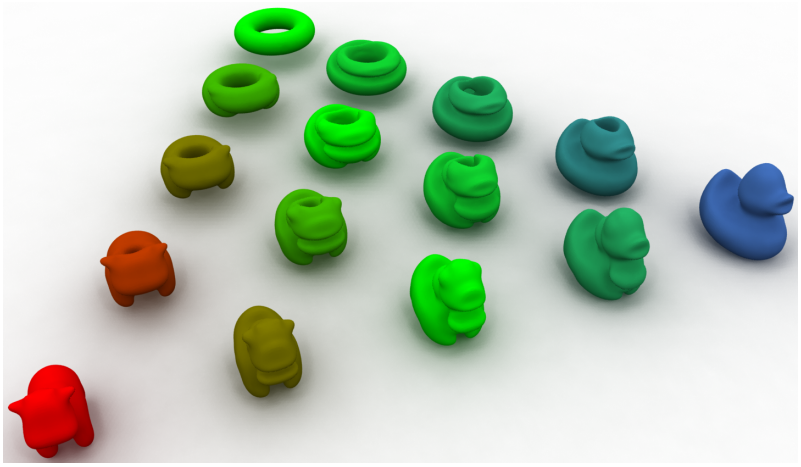

Figure 9. Example of barycenter between shapes computed using optimal transport barycenters of the uniform densities inside the 3 extremal shapes, computed as detailed in [169]. Note that the barycenters are not in general uniform distributions, and we display them as the surface defined by a suitable 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 [109]. 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 [92] 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 [169]. 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 [43]- [44]- [45]- [50]:

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

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

3.2.2. High order DG methods for wave propagation models

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

- **Nodal DG methods for time-domain problems**. For the numerical solution of the time-domain Maxwell equations, we have first proposed a non-dissipative high order DGTD (Discontinuous Galerkin Time-Domain) method working on unstructured conforming simplicial meshes [13]. This DG method combines a central numerical flux function for the approximation of the integral term at the interface of two neighboring elements with a second order leap-frog time integration scheme. Moreover, the local approximation of the electromagnetic field relies on a nodal (Lagrange type) polynomial interpolation method. Recent achievements by the team deal with the extension of these methods towards non-conforming unstructured [10]-[11] and hybrid structured/unstructured meshes [6], their coupling with hybrid explicit/implicit time integration schemes in order to improve their efficiency in the context of locally refined meshes [4]-[20]-[19]. A high order DG method has also been proposed for the numerical resolution of the elastodynamic equations modeling the propagation of seismic waves [2]-[9].
- **Hybridizable DG (HDG) method for time-domain and time-harmonic problems**. For the numerical treatment of the time-harmonic Maxwell equations, nodal DG methods can also be considered [8]. However, such DG formulations are highly expensive, especially for the discretization of 3D problems, because they lead to a large sparse and undefinite linear system of equations coupling all the degrees of freedom of the unknown physical fields. Different attempts have been made in the recent past to improve this situation and one promising strategy has been recently proposed by Cockburn *et al.*[48] 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 [16]-[17].
- **Multiscale DG methods for time-domain problems**. More recently, in collaboration with LNCC in Petropolis (Frédéric Valentin) the framework of the HOMAR assoacite team, we are investigating a family of methods specifically designed for an accurate and efficient numerical treatment of multiscale wave propagation problems. These methods, referred to as Multiscale Hybrid Mixed (MHM) methods, are currently studied in the team for both time-domain electromagnetic and elastodynamic PDE models. They consist in reformulating the mixed variational form of each system into a global (arbitrarily coarse) problem related to a weak formulation of the boundary condition (carried by a Lagrange multiplier that represents e.g. the normal stress tensor in elastodynamic sytems), and a series of small, element-wise, fully decoupled problems resembling to the initial one and related to some well chosen partition of the solution variables on each element. By construction, that methodology is fully parallelizable and recursivity may be used in each local problem as well, making MHM methods belonging to multi-level highly parallelizable methods. Each local problem may be solved using DG or classical Galerkin FE approximations combined with some appropriate time integration scheme (θ-scheme or leap-frog scheme).

3.3. Efficient time integration strategies

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

However, explicit DGTD methods are also constrained by a stability condition that can be very restrictive on highly refined meshes and when the local approximation relies on high order polynomial interpolation. There are basically three strategies that can be considered to cure this computational efficiency problem. The first approach is to use an unconditionally stable implicit time integration scheme to overcome the restrictive constraint on the time step for locally refined meshes. In a second approach, a local time stepping strategy is combined with an explicit time integration scheme. In the third approach, the time step size restriction is overcome by using a hybrid explicit-implicit procedure. In this case, one blends a time implicit and a time explicit schemes where only the solution variables defined on the smallest elements are treated implicitly. The first and third options are considered in the team in the framework of DG [4]-[20]-[19] 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 [15]. 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 [22]. In the context of seismic wave propagation, we are interested by the intrinsic attenuation of the medium [21]. 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 [71].

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 [37]. 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 [39], a wheelbarrow molecule [51], a nano-car [76], a Morse molecule [19], etc. Typically, these designs are optimized using semi-empirical quantum mechanics calculations, such as the semi-empirical ASED+ calculation technique [20].

While impressive, these are but two examples of the nanoscience revolution already impacting numerous fields, including electronics and semiconductors [58], textiles [57], [43], energy [61], food [32], drug delivery [41], [78], chemicals [44], materials [33], the automotive industry [17], aerospace and defense [40], medical devices and therapeutics [35], medical diagnostics [82], etc. According to some estimates, the world market for nanotechnology-related products and services will reach one trillion dollars by 2015 [70]. 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 [84], removing some degrees of freedom (e.g. keeping torsion angles only [56], [77]), coarse-graining [83], [73], [21], [75], multiple time step methods [67], [68], fast multipole methods [36], parallelization [54], averaging [31], multi-scale modeling [29], [26], reactive force fields [28], [87], interactive multiplayer games for predicting protein structures [34], 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 [85], [86].

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 [63], [64], [65], [66], the adaptive multiscale method [60], and the adaptive partitioning of the Lagrangian method [46]. Although these approaches have demonstrated some convincing applications, they all suffer from a number of limitations stemming from the fact that they are either ad hoc methods tuned to fix specific problems (e.g. fix density problems in regions where the level of description changes), or mathematically founded methods that necessitate to "calibrate" potentials so that they can be mixed (i.e. all potentials have to agree on a reference point). In general, multi-scale methods, even when

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

3.4. Research axes

The goal of the NANO-D group is to help current and future designers of *nanosystems*, i.e. systems studied or designed at the atomic scale (whether natural or artificial, independently of the application domain, including structural biology, material science, chemistry, etc.) by developing the **foundations of a software application which will run on a desktop computer, and will allow for efficient analysis, design, modeling and simulation of nanosystems**.

To achieve this, we will be developing a series of **adaptive methods and algorithms** that allow users to focus computational resources on the parts of the models that they want to simulate, and that allow to finely trade between speed and precision.

In parallel, we will develop the architecture of a new desktop application for virtual prototyping of nanosystems, and will integrate all our algorithms into this application. Furthermore, the architecture of this platform will be open, so that independent developers may add modules, for **multiple application domains** (physics, biology, chemistry, materials, electronics, etc.). With this open platform, we will attempt to federate the research performed in computational nanoscience throughout the world.

This application is called **SAMSON: "Software for Adaptive Modeling and Simulation Of Nanosystems"**.

Our two research axes are:

1. **Developing adaptive algorithms for simulating nanosystems**
   - **Defining adaptive Hamiltonians**: In order to be able to perform simulations with good mathematical properties, we are expanding on our recent work on *adaptively restrained Hamiltonians*[23], *i.e.* modified Hamiltonian representations of molecular systems that are able to switch degrees of freedom on and off during a simulation. These will allow us to finely trade between precision and computational performance, by choosing arbitrarily the number of degrees of freedom. Even though we have already obtained some promising results in this domain, our goal is to develop several different simplification methods.
   - **Developing algorithms for incremental potential update**: In order to benefit from performing adaptive particle simulations, we need to develop a series of algorithms that will take advantage of the fact that some (potentially relative) atomic positions are frozen. We have already demonstrated how this is possible for torsion-angle quasi-static simulation of classical bio-molecular force-fields [72], for neighbor search between large rigid molecules [22], and for bond-order reactive force-fields [27]. We are developing new algorithms for incremental neighbor search, energy and force updates corresponding to the adaptive Hamiltonians that we are defining.
2. **Developing algorithms for modeling molecular interactions**
   - **Developing knowledge-driven methods, potentials and algorithms**: Over time, more and more experimental information becomes available. One can use this information to predict and discover new types of molecular interactions and various mechanisms or molecular organization. For example, currently there are more than 50,000 protein structures of a high resolution stored in the Protein Data Bank [25] and over 500,000 structures of small molecules stored in the Cambridge Structural Database [18]. We are developing algorithms for protein-protein interactions and protein-ligand interactions.

- **Developing parametrization algorithms for interaction potentials**: Molecular models typically require their own potential energy function (or a *forcefield*) to be assigned. However, the development of a new potential function is a very difficult and sometimes challenging task [48]. Therefore, we are developing algorithms for automatic parametrization of new potential functions for some particular representations of a molecular system.
- **Developing algorithms for exhaustive sampling**: Some application domains, such as computational docking, cryo-EM rigid-body fitting, etc., require sampling in a low-dimensional space. For such applications it is advantageous to perform an exhaustive search rather than accelerated sampling [69]. Therefore, we are developing fast search methods to perform exhaustive search.

POEMS Project-Team

3. Research Program

3.1. General description

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

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

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

3.2. New schemes for time-domain simulations

Problems of wave propagation naturally arise as problems of evolution and it is necessary to have efficient methods for the calculation of their solution, directly in the time domain. The development and analysis of such methods has been in the past an important part of POEMS activity. Nowadays, there exists a large variety of higher order numerical methods that allow us to solve with good accuracy and in short computational time most classical wave propagation problems. However, when on wishes to deal with real life applications, one has to tackle problems which are complex in many ways: they involve multi-physics, non standard (possibly nonlinear) constitutive laws, highly heterogeneous media with high contrasts of coefficients, complex geometries... In many cases, such problems escape to the direct application of the above mentioned methods and ad hoc dedicated methods have to be designed. Such methods are most often of hybrid nature, which includes domain decomposition methods and subgridding, mixing of integral equations and PDEs, and artificial boundary conditions. In time domain, a particularly challenging issue is the time stability, in particular concerning the coupling of algorithms. To cope with this major difficulty, a key issue (and a kind of graal for numerical analysts) is the development of energy preserving methods which is one of the specificity of the research developed at POEMS in this field.

3.3. Integral equations

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

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

On the other hand, POEMS is developing Fast Boundary Element Methods for 3D acoustics or elastodynamics, with applications to soil-structure interaction, seismology or seismic imaging.

Finally, a posteriori error analysis methodologies and adaptivity for boundary integral equation formulations of acoustic, electromagnetic and elastic wave propagation are investigated, continuing what was intiated during the ANR project RAFFINE.

3.4. Domain decomposition methods

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

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

One ANR project (NonLocalDD) supports this research.

3.5. Wave propagation in complex media

Our objective is first to develop efficient numerical approaches for the propagation of waves in heterogeneous media, taking into account their complex microstructure.

We aim on one hand to improve homogenized modeling of periodic media, by deriving enriched boundary conditions (or transmission conditions if the periodic structure is embedded in a homogeneous matrix) which take into account the boundary layer phenomena. On the other hand, we like to develop multi-scale numerical methods when the assumption of periodicity on the spatial distribution of the heterogeneities is relaxed, or even completely lost. The general idea consists in a coupling between a macroscopic solver, based on a coarse mesh, with some microscopic representation of the field. This latter can be obtained by a numerical microscopic solver or by an analytical asymptotic expansion. This leads to two very different approaches which may be relevant for very different applications.

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

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

3.6. Spectral theory and modal approaches

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

Then, we would like to go further in proving the absence of localized modes in non uniform open waveguides. An original approach has been successfully applied to the scalar problem of a waveguides junctions or bent waveguides. The challenge now is to extend these ideas to vectorial problems (for applications to electromagnetism or elastodynamics) and to junctions of periodic waveguides.

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

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

3.7. Inverse problems

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

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

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

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

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 on the recent breakthrough proposed by C. Cancès & C. Guichard [7], [21] 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 [75] 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 [68], [90]).

Recently, C. Chainais-Hillairet and co-authors [3], [8] and [69] developed a strategy based on the control of the numerical counterpart of the physical entropy to develop and analyze AP numerical methods. In particular, these methods show great promises for capturing accurately the behavior of the solutions to dissipative problems when some physical parameter is small with respect to the discretization characteristic parameters, or in the long-time asymptotic. Since it requires the use of nonlinear test functions in the analysis, strong restrictions on the physics (isotropic problems) and on the mesh (Cartesian grids, Voronoï boxes...) are required in [3], [8] and [69]. The schemes proposed in [7] and [21] 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* [7] with the methodology of [3], [8], [69] would provide schemes that are robust both with respect to the meshes and to the parameters. Therefore, they would be also robust under adaptive mesh refinement.

3.1.3. Design and stability analysis of numerical methods for mixture problems

We aim at extending the range of the `NS2DDV-M` software by introducing new physical models, like for instance the Kazhikov and Smagulov model [87]. This will require a theoretical study for proving the existence of weak solutions to this model. Then, we will need to design numerical schemes to approximate these models and study their stability. We will also study their convergence following the path proposed in [83], [88].

3.2. Optimizing the computational efficiency

3.2.1. High order nonlinear numerical methods

The numerical experiments carried out in [7] 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) [78].

Concerning the inhomogeneous fluid models, we aim to investigate new methods for the mass equation resolution. Indeed, we aim at increasing the accuracy while maintaining some positivity-like properties and the efficiency for a wide range of physical parameters. To this end, we will consider *residual distribution* (RD) schemes, that appear as an alternative to finite volume methods. RD schemes enjoy very compact stencils. Therefore, their extension from 2D to 3D yield reasonable difficulties. These methods appeared twenty years ago, but recent extensions to unsteady problems [91], [84], with high-order accuracy [54], [53], or for parabolic problems [51], [52] make them very competitive. Relying on these breakthroughs, we aim at designing new RD schemes for fluid mixture models with high-order accuracy while preserving the positivity of the solutions.

3.2.2. A posteriori error control

The question of the *a posteriori* error estimators will also have to be addressed in this optimization context. Since the pioneering papers of Babuska and Rheinboldt more than thirty years ago [59], *a posteriori* error estimators have been widely studied. We will take advantage of the huge corresponding bibliography database in order to optimize our numerical results.

For example, we would like to generalize the results we derived for the harmonic magnetodynamic case (e.g. [10] and [70]) to the temporal magnetodynamic one, for which space/time *a posteriori* error estimators have to be developed. A space/time refinement algorithm should consequently be proposed and tested on academic as well as industrial benchmarks.

We also want to develop *a posteriori* estimators for the variable density Navier-Stokes model or some of its variants. To do so, several difficulties have to be tackled: the problem is nonlinear, unsteady, and the numerical method [5], [6] we developed combines features from finite elements and finite volumes. Fortunately, we do not start from scratch. Some recent references are devoted to the unsteady Navier-Stokes model in the finite element context [63], [96]. In the finite volume context, recent references deal with unsteady convection-diffusion equations [95], [57], [73] and [67]. 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 [82]. This reduces the $O(N^2)$ naïve computational cost of the interactions to $O(N \log N)$, allowing numerical simulations involving millions of individuals.

APICS Project-Team

3. Research Program

3.1. Introduction

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

Practice is not nearly as simple, for f is only measured pointwise in the pass-band of the system which makes the problem ill-posed [71]. 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 [77] 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 [35].

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 [73], [58]. 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 5.2.2 .

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 [63] 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] [32], [81]. 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* [70]. In the two steps approach previously described, we implicitly removed this indeterminacy by requiring in step 1 that the measure be supported on the boundary (because we seek a function holomorphic throughout the right half-space), and by requiring in step 2 that the measure be discrete in the left half-plane (in fact: a sum of point masses $\sum_1^n a_j \delta_{z_j}$). The discreteness assumption also prevails in 3-D inverse source problems, see Section 4.3 . Conditions that ensure uniqueness of the solution to the inverse potential problem are part of the so-called regularizing assumptions which are needed in each case to derive efficient algorithms.

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

Along these lines, Apics advocates the use of steps 1 and 2 above, along with some singularity analysis, to approach issues of nondestructive control in 2-D and 3-D [2], [42], [46]. 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 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.

Apics is reaching the end of its 12 years life cycle. A reorganization of the team and of some of its research themes is under way through the project proposal FACTAS.

3.2. Range of inverse problems

3.2.1. Elliptic partial differential equations (PDE)

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

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 [56], [59].

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* [62]. 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 the conjugate-Beltrami equation, which is an interesting topic by itself. For Sobolev-smooth coefficients of exponent greater than 2, they were investigated in [5], [36]. The case of the critical exponent 2 is treated in [31], 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 [32] where we address the uniqueness issue in the classical Robin inverse problem on a Lipschitz domain of $\Omega \subset \mathbb{R}^n$, $n \geq 2$, with uniformly bounded Robin coefficient, L^2 Neumann data and conductivity of Sobolev class $W^{1,r}(\Omega)$, $r > n$. We show that uniqueness of the Robin coefficient on a subset of the boundary, given Cauchy data on the complementary part, does hold in dimension $n = 2$, thanks to a unique continuation result, but needs not hold in higher dimension. In higher dimension, this raises an open issue on harmonic gradients, namely whether the positivity of the Robin coefficient is compatible with identical vanishing of the boundary gradient on a subset of positive measure.

The 3-D version of step 1 in Section 3.1 is another subject investigated by Apics: to recover a harmonic function (up to an additive constant) in a ball or a half-space from partial knowledge of its gradient. This prototypical inverse problem (*i.e.* inverse to the Cauchy problem for the Laplace equation) often recurs in electromagnetism. At present, Apics is involved with solving instances of this inverse problem arising in two fields, namely medical imaging *e.g.* for electroencephalography (EEG) or magneto-encephalography (MEG), and paleomagnetism (recovery of rocks magnetization) [2], [38], see Section 5.1 . In this connection, we collaborate with two groups of partners: Athena Inria project-team, CHU La Timone, and BESA company on the one hand, Geosciences Lab. at MIT and Cerege CNRS Lab. on the other hand. The question is considerably more difficult than its 2-D counterpart, due mainly to the lack of multiplicative structure for harmonic gradients. Still, substantial progress has been made over the last years using methods of harmonic analysis and operator theory.

The team is further concerned with 3-D generalizations and applications to non-destructive control of step 2 in Section 3.1 . A typical problem is here to localize inhomogeneities or defaults such as cracks, sources or occlusions in a planar or 3-dimensional object, knowing thermal, electrical, or magnetic measurements on the boundary. These defaults can be expressed as a lack of harmonicity of the solution to the associated Dirichlet-Neumann problem, thereby posing an inverse potential problem in order to recover them. In 2-D, finding an optimal discretization of the potential in Sobolev norm amounts to solve a best rational approximation problem, and the question arises as to how the location of the singularities of the approximant (*i.e.* its poles) reflects the location of the singularities of the potential (*i.e.* the defaults we seek). This is a fairly deep issue in approximation theory, to which Apics contributed convergence results for certain classes of fields expressed as Cauchy integrals over extremal contours for the logarithmic potential [6], [39], [53]. Initial schemes to locate cracks or sources *via* rational approximation on planar domains were obtained this way [42], [46], [56]. It is remarkable that finite inverse source problems in 3-D balls, or more general algebraic surfaces, can be approached using these 2-D techniques upon slicing the domain into planar sections [7], [43]. More precisely, each section cuts out a planar domain, the boundary of which carries data which can be proved to match an algebraic function. The singularities of this algebraic function are not located at the 3-D sources, but are related to them: the section contains a source if and only if some function of the singularities in that section meets a relative extremum. Using bisection it is thus possible to determine an extremal place along all sections parallel to a given plane direction, up to some threshold which has to be chosen small enough that one does not miss a source. This way, we reduce the original source problem in 3-D to a sequence of inverse poles and branchpoints problems in 2-D. This bottom line generates a steady research activity within Apics, and again applications are sought to medical imaging and geosciences, see Sections 4.3 , 4.2 and 5.1 .

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

3.2.2. Systems, transfer and scattering

Participants: Laurent Baratchart, 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 [9] for details.
2. A stable rational approximation of appropriate degree to the model obtained in the previous step is performed. For this, a descent method on the compact manifold of inner matrices of given size and degree is used, based on an original parametrization of stable transfer functions developed within the team [27], [9].

3. Realizations of this rational approximant are computed. To be useful, they must satisfy certain constraints imposed by the geometry of the device. These constraints typically come from the coupling topology of the equivalent electrical network used to model the filter. This network is composed of resonators, coupled according to some specific graph. This realization step can be recast, under appropriate compatibility conditions [57], as solving a zero-dimensional multivariate polynomial system. To tackle this problem in practice, we use Gröbner basis techniques and continuation methods which team up in the Dedale-HF software (see Section 3.4.1).

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

Apics also investigates issues pertaining to design rather than identification. Given the topology of the filter, a basic problem in this connection is to find the optimal response subject to specifications that bear on rejection, transmission and group delay of the scattering parameters. Generalizing the classical approach based on Chebyshev polynomials for single band filters, we recast the problem of multi-band response synthesis as a generalization of the classical Zolotarev min-max problem for rational functions [26] [8]. Thanks to quasi-convexity, the latter can be solved efficiently using iterative methods relying on linear programming. These were implemented in the software easy-FF (see easy-FF). Currently, the team is engaged in the synthesis of more complex microwave devices like multiplexers and routers, which connect several filters through wave guides. Schur analysis plays an important role here, because scattering matrices of passive systems are of Schur type (*i.e.* contractive in the stability region). The theory originates with the work of I. Schur [76], 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 [28]. Dwelling on this, Apics contributed differential parametrizations (atlases of charts) of lossless matrix functions [27], [72], [67] which are fundamental to our rational approximation software RARL2 (see Section 3.4.4). Schur analysis is also instrumental to approach de-embedding issues, and provides one with considerable insight into the so-called matching problem. The latter consists in maximizing the power a multiport can pass to a given load, and for reasons of efficiency it is all-pervasive in microwave and electric network design, *e.g.* of antennas, multiplexers, wifi cards and more. It can be viewed as a rational approximation problem in the hyperbolic metric, and the team presently deals with this hot topic using contractive interpolation with constraints on boundary peak points, within the framework of the (defense funded) ANR Cocoram, see Sections 5.2 and 7.2.1 .

In recent years, our attention was driven by CNES and UPV (Bilbao) to questions about stability of high-frequency amplifiers. Contrary to previously discussed devices, these are *active* components. The response of an amplifier can be linearized around a set of primary current and voltages, and then admittances of the corresponding electrical network can be computed at various frequencies, using the so-called harmonic balance method. The initial goal is to check for stability of the linearized model, so as to ascertain existence of a well-defined working state. The network is composed of lumped electrical elements namely inductors, capacitors, negative *and* positive reactors, transmission lines, and controlled current sources. Our research so far has focused on describing the algebraic structure of admittance functions, so as to set up a function-theoretic framework where the two-steps approach outlined in Section 3.1 can be put to work. The main discovery is that the unstable part of each partial transfer function is rational and can be computed by analytic projection, see Section 5.3 . 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 [41], [44], [50], the solution to this convex infinite-dimensional optimization problem can be obtained when $p \neq 1$ upon iterating with respect to a Lagrange parameter the solution to spectral equations for appropriate Hankel and Toeplitz operators. These spectral equations involve the solution to the special case $K = T$ of (P), which is a standard extremal problem [65]:

> (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 [45], [18]. In this form, the problem comes close to (but still is different from) H^∞ frequency optimization used in control [68], [75]. One can also impose bounds on the real or imaginary part of $g - \psi$ on $T \setminus K$, which is useful when considering Dirichlet-Neumann problems, see [19].

The analog of Problem (P) on an annulus, K being now the outer boundary, can be seen as a means to regularize a classical inverse problem occurring in nondestructive control, namely to recover a harmonic function on the inner boundary from Dirichlet-Neumann data on the outer boundary (see Sections 3.2.1 , 4.3 , 5.1.3). 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: $\overline{\partial} f = \nu \overline{\partial f}$ [69], which are studied for $1 < p < \infty$ in [5], [31], [36] and [60]. 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 [62].

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 [79]. 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 [41] to the 3-D case, using a generalization of Toeplitz operators. The case of the shell was motivated by applications to the processing of EEG data. An important ingredient is a refinement of the Hodge decomposition, that we call the *Hardy-Hodge* decomposition, allowing us to express a $\mathbb{R}^n$-valued vector field in $L^p(S)$, $1 < p < \infty$, as the sum of a vector field in $H^p(B)$, a vector field in $H^p(\mathbb{R}^n \setminus \overline{B})$, and a tangential divergence free vector field on S; the space of such divergence-free fields is denoted by $D(S)$. If $p = 1$ or $p = \infty$, L^p must be replaced by the real Hardy space or the space of functions with bounded mean oscillation. More generally this decomposition, which is valid on any sufficiently smooth surface (see Section 5.1), seems to play a fundamental role in inverse potential problems. In fact, it was first introduced formally on the plane to describe silent magnetizations supported in $\mathbb{R}^2$ (*i.e.* those generating no field in the upper half space) [38].

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

> (P_2) Let $1 \leq p \leq \infty$ 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 [74].

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 [74].

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 [33]. 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 [47], [49]. Based on this work, uniqueness or asymptotic uniqueness of the approximant was proved for certain classes of functions like transfer functions of relaxation systems (*i.e.* Markov functions) [51] and more generally Cauchy integrals over hyperbolic geodesic arcs [54]. These are the only results of this kind. Research by Apics on this topic remained dormant for a while by reasons of opportunity, but revisiting the work [29] 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 [50]. 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 [55], [52], and is used in an essential manner to assess the behavior of poles of best approximants to functions with branched singularities, which is of particular interest for inverse source problems (*cf.* Sections 3.4.2 and 5.1).

In higher dimensions, the analog of Problem (P_N) is best approximation of a vector field by gradients of discrete potentials generated by N point masses. This basic issue is by no means fully understood, and it is an exciting field of research. It is connected with certain generalizations of Toeplitz or Hankel operators, and with constructive approaches to so-called weak factorizations for real Hardy functions [61].

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 [66]. 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 [37], [40].

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 [33] and mentioned in Section 3.3.2.1 generalizes to the matrix-valued situation [64]. 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 ([27], [67], [72]). Some of these parametrizations are also interesting to compute realizations and achieve filter synthesis ([67], [72]). 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 [48]. Matrix-valued Markov functions are the only known example beyond this one [30].

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

3.3.3. Behavior of poles of meromorphic approximants

Participant: Laurent Baratchart.

We refer here to the behavior of poles of best meromorphic approximants, in the L^p-sense on a closed curve, to functions f defined as Cauchy integrals of complex measures whose support lies inside the curve. Normalizing the contour to be the unit circle T, we are back to Problem (P_N) in Section 3.3.2.1 ; invariance of the latter under conformal mapping was established in [46]. Research so far has focused on functions whose singular set inside the contour is polar, meaning that the function can be continued analytically (possibly in a multiple-valued manner) except over a set of logarithmic capacity zero.

Generally speaking in approximation theory, assessing the behavior of poles of rational approximants is essential to obtain error rates as the degree goes large, and to tackle constructive issues like uniqueness. However, as explained in Section 3.2.1 , the original twist by Apics is to consider this issue also as a means to extract information on singularities of the solution to a Dirichlet-Neumann problem. The general theme is thus: *how do the singularities of the approximant reflect those of the approximated function?* This approach to inverse problem for the 2-D Laplacian turns out to be attractive when singularities are zero- or one-dimensional (see Section 4.3). It can be used as a computationally cheap initial condition for more precise but much heavier numerical optimizations which often do not even converge unless properly initialized. As regards crack detection or source recovery, this approach boils down to analyzing the behavior of best meromorphic approximants of given pole cardinality to a function with branch points, which is the prototype of a polar singular set. For piecewise analytic cracks, or in the case of sources, we were able to prove ([6], [46], [39]), that the poles of the approximants accumulate, when the degree goes large, to some extremal cut of minimum weighted logarithmic capacity connecting the singular points of the crack, or the sources [42]. Moreover, the asymptotic density of the poles turns out to be the Green equilibrium distribution on this cut in D, therefore it charges the singular points if one is able to approximate in sufficiently high degree (this is where the method could fail, because high-order approximation requires rather precise data).

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

It is remarkable that inverse source problems inside a sphere or an ellipsoid in 3-D can be approached with such 2-D techniques, as applied to planar sections, see Section 5.1 . The technique is implemented in the software FindSources3D, see Section 3.4.2 .

3.4. Software tools of the team

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

3.4.1. DEDALE-HF

SCIENTIFIC DESCRIPTION

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

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

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

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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 [7].

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.

- Participants: Juliette Leblond, Maureen Clerc (team Athena, Inria Sophia), Jean-Paul Marmorat, Théodore Papadopoulo (team Athena).
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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.

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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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BIPOP Project-Team

3. Research Program

3.1. Dynamic non-regular systems

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

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

$$\begin{cases} \dot{x} = f(x,u,\lambda)\,, \\ 0 \le y \perp \lambda \ge 0\,, \\ g(y,\lambda,x,u,t) = 0\,, \\ \text{re-initialization law of the state } x(\cdot), \end{cases} \tag{21}$$

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

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

Thus, the 2nd and 3rd lines in (1) define the modes of the hybrid systems, as well as the conditions under which transitions occur from one mode to another. The 4th line defines how transitions are performed by the state x. There are several other formalisms which are quite related to complementarity. See [7], [8], [17] for a survey on models and control issues in nonsmooth mechanical systems.

3.2. Nonsmooth optimization

optimization, numerical algorithms.

$\Longrightarrow$*The optimization scientific activity in BIPOP is no longer existing after Jérôme Malick left BIPOP to lead the DAO team in the Laboratoire Jean Kuntzman.*

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 [32]), with improvements due to the "Chicago school", Bliss [24] during the first part of the 20th century, and by the notion of relaxed problem and generalized solution (Young [37]).

Trajectory optimization really started with the spectacular achievement done by Pontryagin's group [36] 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 [28], Leitmann [34], Lee and Markus [33], Ioffe and Tihomirov [31]).

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 [29]. The theoretical contributions in this direction did not cease growing, see the books by Barles [22] and Bardi and Capuzzo-Dolcetta [21].

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 [30], Bonnans [25]. 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 [27]. 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 [26].

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) eventually 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 might have fixed delays, time-varying delays, distributed delays ...

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

- Robustness/fragility of biological systems

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

  However, for other biological systems, the notion of robustness may be different and this question is still in its infancy (see, e.g. [70]). 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], [71].

- Predictive control

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

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

GECO Project-Team

3. Research Program

3.1. Geometric control theory

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

Geometric control theory provides a viewpoint and several tools, issued in particular from differential geometry, to tackle typical questions arising in the control framework: controllability, observability, stabilization, optimal control... [9], [43] The geometric control approach is particularly well suited for systems involving nonlinear and nonholonomic phenomena. We recall that nonholonomicity refers to the property of a velocity constraint that is not equivalent to a state constraint.

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

We recall that

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

At the core of control design is then the notion of motion planning. Among the motion planning methods, a preeminent role is played by those based on the Lie algebra associated with the control system ([63], [50], [56]), those exploiting the possible flatness of the system ([37]) and those based on the continuation method ([75]). Optimal control is clearly another method for choosing a control law connecting two states, although it generally introduces new computational and theoretical difficulties.

Control systems with special structure, which are very important for applications are those for which the controls appear linearly. When the controls are not bounded, this means that the admissible velocities form a distribution in the tangent bundle to the state manifold. If the distribution is equipped with a smoothly varying norm (representing a cost of the control), the resulting geometrical structure is called *sub-Riemannian*. Sub-Riemannian geometry thus appears as the underlying geometry of the nonholonomic control systems, playing the same role as Euclidean geometry for linear systems. As such, its study is fundamental for control design. Moreover its importance goes far beyond control theory and is an active field of research both in differential geometry ([62]), geometric measure theory ([38], [13]) and hypoelliptic operator theory ([25]).

Other important classes of control systems are those modeling mechanical systems. The dynamics are naturally defined on the tangent or cotangent bundle of the configuration manifold, they have Lagrangian or Hamiltonian structure, and the controls act as forces. When the controls appear linearly, the resulting model can be seen somehow as a second-order sub-Riemannian structure (see [30]).

The control design topics presented above naturally extend to the case of distributed parameter control systems. The geometric approach to control systems governed by partial differential equations is a novel subject with great potential. It could complement purely analytical and numerical approaches, thanks to its more dynamical, qualitative and intrinsic point of view. An interesting example of this approach is the paper [10] about the controllability of Navier–Stokes equation by low forcing modes.

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 :

$$\left\{\begin{array}{rcl} X_{k+1} & = & F\ X_k + V_{k+1} \\ Y_k & = & H\ X_k + W_k \end{array}\right. , \tag{22}$$

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

$$\det\ (F-\lambda\ I)=0,\quad (F-\lambda\ I)\ \phi_\lambda=0,\quad \varphi_\lambda\stackrel{\Delta}{=}H\ \phi_\lambda \tag{23}$$

The (canonical) parameter vector in that case is :

$$\theta\stackrel{\Delta}{=}\left(\begin{array}{c}\Lambda\\ \mathrm{vec}\Phi\end{array}\right) \tag{24}$$

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

Subspace-based methods is the generic name for linear systems identification algorithms based on either time domain measurements or output covariance matrices, in which different subspaces of Gaussian random vectors play a key role [62].

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

$$\mathcal{H}_{p+1,q} \triangleq \begin{pmatrix} R_1 & R_2 & \vdots & R_q \\ R_2 & R_3 & \vdots & R_{q+1} \\ \vdots & \vdots & \vdots & \vdots \\ R_{p+1} & R_{p+2} & \vdots & R_{p+q} \end{pmatrix} \triangleq \text{Hank}\left(R_i\right) \tag{25}$$

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 :

$$\begin{array}{rcl} R_i & = & HF^{i-1}G \\ \mathcal{H}_{p+1,q} & = & \mathcal{O}_{p+1}(H,F)\ \mathcal{C}_q(F,G) \end{array} \tag{26}$$

where:

$$\mathcal{O}_{p+1}(H,F) \triangleq \begin{pmatrix} H \\ HF \\ \vdots \\ HF^p \end{pmatrix} \quad \text{and} \quad \mathcal{C}_q(F,G) \triangleq (G\ FG\ \cdots\ F^{q-1}G) \tag{27}$$

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:

$$\mathcal{O}_{p+1}(\theta) = \begin{pmatrix} \Phi \\ \Phi\Delta \\ \vdots \\ \Phi\Delta^p \end{pmatrix} \tag{28}$$

where $\Delta \triangleq \text{diag}(\Lambda)$, 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:

$$\mathcal{O}_{p+1}(\theta_0) \text{ and } \mathcal{H}_{p+1,q} \text{ have the same left kernel space.} \tag{29}$$

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:

$$U^T\, U = I_s \text{ and } U^T\, \mathcal{O}_{p+1}(\theta_0) = 0 \tag{30}$$

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:

$$U(\theta_0)^T\, \mathcal{H}_{p+1,q} = 0 \tag{31}$$

3.1.2.1. Residual associated with subspace identification.

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

$$\widehat{\mathcal{H}}_{p+1,q} \triangleq \text{Hank}\left(\widehat{R}_i\right), \quad \widehat{R}_i \triangleq 1/(N-i) \sum_{k=i+1}^{N} Y_k\, Y_{k-i}^T \tag{32}$$

and to define the residual vector:

$$\zeta_N(\theta_0) \triangleq \sqrt{N}\ \text{vec}\left(U(\theta_0)^T\, \widehat{\mathcal{H}}_{p+1,q}\right) \tag{33}$$

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 [56] that the residual is asymptotically Gaussian :

$$\zeta_N \xrightarrow[N \to \infty]{} \begin{cases} \mathcal{N}(0, \Sigma) & \text{under } \mathbf{P}_{\theta_0} \ , \\ \\ \mathcal{N}(\mathcal{J}\,\eta, \Sigma) & \text{under } \mathbf{P}_{\theta_0 + \eta/\sqrt{N}} \ , \end{cases} \tag{34}$$

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 :

$$\chi^2 = \overline{\zeta}^{\,T}\, \mathbf{F}^{-1}\, \overline{\zeta} \gtrless \lambda \ . \tag{35}$$

where

$$\overline{\zeta} \triangleq \mathcal{J}^T\, \Sigma^{-1}\, \zeta_N \quad \text{and} \quad \mathbf{F} \triangleq \mathcal{J}^T\, \Sigma^{-1}\, \mathcal{J} \tag{36}$$

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 [55].

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

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

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

$$\chi^2_\Phi = \zeta^T\, \Sigma^{-1}\, \mathcal{J}\, \mathcal{J}_{\Phi\theta}\, (\mathcal{J}^T_{\Phi\theta}\, \mathcal{J}^T\, \Sigma^{-1}\, \mathcal{J}\, \mathcal{J}_{\Phi\theta})^{-1}\, \mathcal{J}^T_{\Phi\theta}\, \mathcal{J}^T\, \Sigma^{-1}\, \zeta \gtrless \lambda \ . \tag{37}$$

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

3.2. Thermal methods

3.2.1. Infrared thermography and heat transfer

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

3.2.1.1. Infrared radiation

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

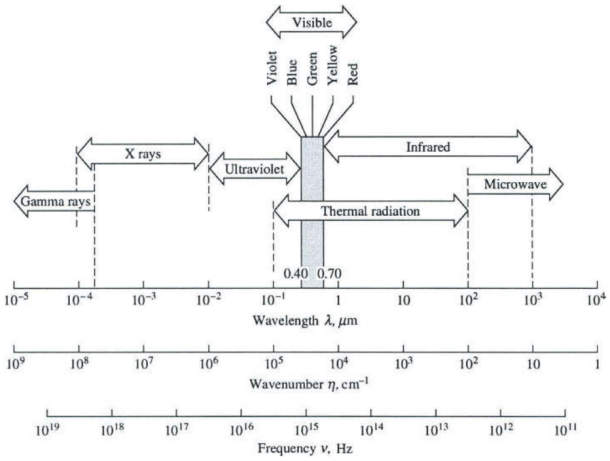

Figure 1. Electromagnetic spectrum - Credit MODEST, M.F. (1993). Radiative Heat Transfer. Academic Press.

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

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

Band name	**wavelength**	**Uses ⟍ 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).

$$M^o_{\lambda,T} = \frac{C_1 \lambda^{-5}}{\exp^{\frac{C_2}{\lambda T}} - 1} \tag{38}$$

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

$$\begin{aligned} C_1 &= 2hc^2\pi \\ C_2 &= h\frac{c}{k} \end{aligned} \tag{39}$$

with

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

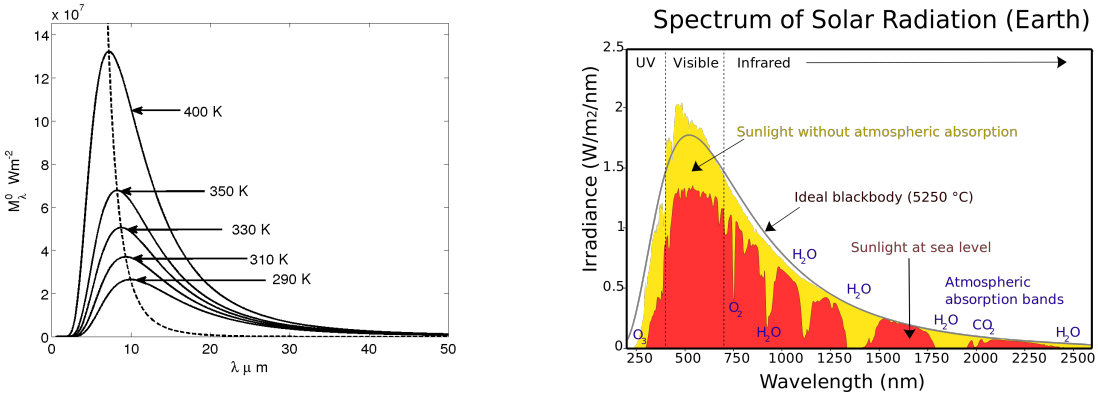

Figure 2. Left: Plank's law at various temperatures - Right: Energy spectrum of the atmosphere

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

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

3.2.1.2. Infrared Thermography

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

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

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

3.2.2. Heat transfer theory

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

$$\varphi = k\nabla T \quad X \in \Omega \tag{40}$$

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

$$\rho C \frac{\partial T(X,t)}{\partial t} = \nabla \cdot (k \nabla T) + P \quad X \in \Omega \tag{41}$$

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).

$$\varphi = k \nabla T \cdot n = \underbrace{h \left(T_{fluid} - T_{Boundarie}\right)}_{\text{Convection}} + \underbrace{\epsilon \sigma_s \left(T^4_{environement} - T^4_{Boundary}\right)}_{\text{Radiation}} + \varphi_0 \quad X \in \partial\Omega \tag{42}$$

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

3.2.3. Inverse model for parameters estimation

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

$$AP = b \tag{43}$$

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).

$$P = A^{-1} b \tag{44}$$

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

$$AP \approx \mathcal{M} \tag{45}$$

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.

$$min_P \left(\|AP - \mathcal{M}\|^2 \right) = min_P \left(\mathcal{F} \right) \tag{46}$$

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

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

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

$$\nabla \mathcal{F}(P) = 2 \left[-\frac{\partial A P^T}{\partial P} \right] \left[AP - \mathcal{M} \right] = 2 J(P)^T \left[AP - \mathcal{M} \right] \tag{47}$$

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

$$P^{k+1} = P^k + \left[\left(J^k \right)^T J^k + \mu^k \Omega^k \right]^{-1} \left(J^k \right)^T \left[\mathcal{M} - A(P^k) \right] \tag{48}$$

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], [61]. 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 [63], [59]. 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.

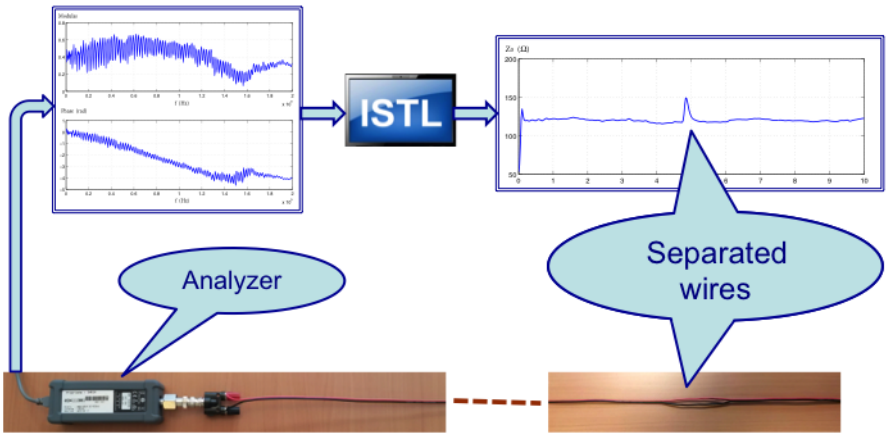

Figure 3. Inverse scattering software (ISTL) for cable soft fault diagnosis.

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 [60]

$$\begin{aligned} &\frac{\partial}{\partial z}V(t,z) + L(z)\frac{\partial}{\partial t}I(t,z) + R(z)I(t,z) = 0 \\ &\frac{\partial}{\partial z}I(t,z) + C(z)\frac{\partial}{\partial t}V(t,z) + G(z)V(t,z) = 0 \end{aligned} \tag{49}$$

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

$$V(t,a) = V_s(t) - R_s I(t,a). \tag{50}$$

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

$$V(t,b) \quad = R_L I(t,b). \tag{51}$$

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 [58]. The visionary idea of applying this theory to solving the cable inverse problem goes also back to the 1980s [57]. After having completed some theoretic results directly linked to practice [14], [61], 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

$$\begin{aligned} \nu_1(\omega,x) &= \frac{1}{2}\left[Z_0^{-\frac{1}{2}}(x)U(\omega,x) - Z_0^{\frac{1}{2}}(x)I(\omega,x)\right] \\ \nu_2(\omega,x) &= \frac{1}{2}\left[Z_0^{-\frac{1}{2}}(x)U(\omega,x) + Z_0^{\frac{1}{2}}(x)I(\omega,x)\right] \end{aligned} \tag{52}$$

with

$$Z_0(x) = \sqrt{\frac{L(x)}{C(x)}}. \tag{53}$$

These transformations lead to the Zakharov-Shabat equations

$$\begin{aligned} \frac{d\nu_1(\omega,x)}{dx} + ik\nu_1(\omega,x) &= q^*(x)\nu_1(\omega,x) + q^+(x)\nu_2(\omega,x) \\ \frac{d\nu_2(\omega,x)}{dx} - ik\nu_2(\omega,x) &= q^-(x)\nu_1(\omega,x) - q^*(x)\nu_2(\omega,x) \end{aligned} \tag{54}$$

with

$$\begin{aligned} q^{\pm}(x) &= -\frac{1}{4}\frac{d}{dx}\left[ln\frac{L(x)}{C(x)}\right] \mp \frac{1}{2}\left[\frac{R(x)}{L(x)} - \frac{G(x)}{C(x)}\right] \\ &= -\frac{1}{2Z_0(x)}\frac{d}{dx}Z_0(x) \mp \frac{1}{2}\left[\frac{R(x)}{L(x)} - \frac{G(x)}{C(x)}\right] \\ q^{*}(x) &= \frac{1}{2}\left[\frac{R(x)}{L(x)} + \frac{G(x)}{C(x)}\right]. \end{aligned} \tag{55}$$

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

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

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

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

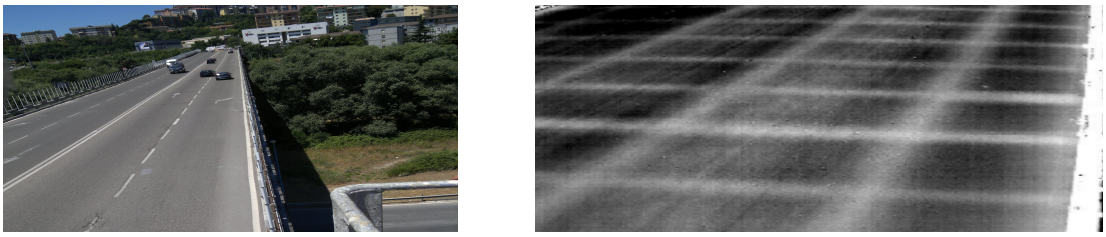

Figure 4. Left: Image in the visible spectrum of the deck surface - Right: PCT result on a bridge deck

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

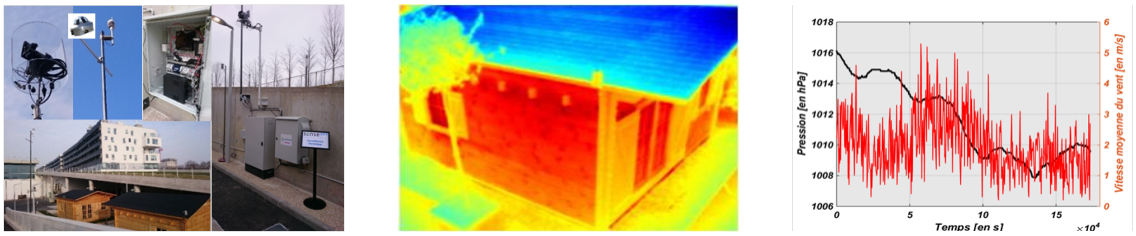

Figure 5. Various view and results of the SenseCity experimentation site - (site and hardware view, IR imaging, Environmental Monitoring)

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 implicated in the development of the 5th Generation Road.

Most of the innovations featured in R5G are now mature, for example communication and few solutions for energy exchange between the infrastructure, the vehicle and the network manager; recyclable materials with the potential for self-diagnosis and repair, a pavement surface that remains permanently optimal irrespective of climatic variations… Nevertheless, implementing them on an industrial scale at a reasonable cost still represents a real challenge. Consultation with the stakeholders (researchers, industry, road network owners 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.

3.1.1. 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. 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".

3.1.2. 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.

3.1.3. 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], [41], [29], 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 .

3.1.4. 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 [59], [72].

3.1.5. 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 [48] or [18], or —although this research has not been active very recently— the study [69] of dynamic feedback and the so-called "flatness" property [62].

3.2. Optimal Control and its Geometry

Let us detail our research program concerning optimal control, evoked in section 3.1.3 . 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 (not all direction can be the tangent of a fesable trajectory 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.

3.2.1. 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 extremal 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 [75], [30], [31] and [49] 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 [40], followed by the *HamPath* [51] 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.* [52] and [37]).

Recently, computation of conjugate points was conducted in [16], [2] 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, and some additional sign conditions must be checked for local minimality, see more in [63]. 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 [28]. 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 [56]).

The cut locus is a central object in Riemannian geometry, control and optimal transport. This is the motivation for the 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. The first one took place during the summer, 2016, in Bangkok; the second one will take place the first week of September, 2018, in Sapporo.

3.2.2. 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 Section 3.4), and/or reduction, some more difficult optimal control problems lead to a Riemann or Finsler geometry

problem, that have been much studied and known facts from these areas are useful. On the other hand, optimal control, mostly the Hamiltonian setting, brings a fresh viewpoint on problems in Riemann and Finsler geometry.

On Riemaniann 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 [61], [60]. The analysis in the oblate geometry [38] was completed in [54] 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 3.4 and 4.1) with L^2-minimization yields a Riemannian metric, thoroughly computed in [35] together with its geodesic flow; in reduced dimension, its conjugate and cut loci were computed in [39] with Japanese Riemaniann geometers. Averaging the same systems for minimum time yields a Finsler Metric, as noted in [34]. In [47], the geodesic convexity properties of these two types of metrics were compared. When perturbation (other than the control) are considered, they introduce a "drift", *i.e.* the Finsler metric is no longer symmetric.

3.2.3. 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 [66] 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 [33], 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 that 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.

3.2.4. Singularities

The analysis of singularities in optimal control yields some more interplay with Hamiltonian dynamics. The Hamiltonian setting, much more than the Lagrangian one used in Riemannian geometry, is instrumental to treat such degeneracies. In fact, the latter do not really create singularities in the Pontryagin Maximum Principle equations. Almost-Riemannian metrics on the two-sphere appear after averaging the Pontryagin Maximum Principle for a quadratic cost (these metrics on the two-sphere are thoroughly described, with their degenracies, in [36]), or in the control of a quantum system with Ising coupling of three spins [45].

Another example comes from the analysis of singularities arising in minimum time systems. Consider a control affine system in dimension four with control on the disc such that the controlled fields together with their first order Lie brackets with the drift have full rank. There is a natural stratification of the codimension two singular set in the cotangent bundle leading to a local classification of extremals in terms of singular and bang arcs. This analysis was done in [52] using the nilpotent model, and extended in [27] by interpreting the singularities of the extremal flow as equilibrium points of a regularized dynamics to prove the continuity of the flow. One can actually treat these singularities as connections of pairs of normally hyperbolic invariant manifolds in order to find a suitable stratification of the flow and prove finer regularity properties. Another issue is to be able to give global bounds on the number of these heteroclinic connections. This work in progress is part of M. Orieux PhD thesis in collaboration with J. Féjoz at U. Paris-Dauphine.

3.2.5. 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 [43], 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 Vinter's group [79], [63] 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 [79], [63].

Another question relevant to locomotion is: how minimizing is it to use periodic deformations ? 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 are 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]).

3.2.6. 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 5.1) 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 transporte measure. This topic attracted renewed attention in the last decade, and has ongoing applications of many types, see section 4.5 . Matching optimal transport with geometric control theory is one originality of our team. Work in the team has been concerned with optimal transport originating from Riemannian geometry ([61] gives strong conditions for continuity of the transport map, [38], [54] checks these conditions on ellipsoids, [60] studies them on more general Riemannian manifolds), sub-Riemannian geometry (see section 6.2.2 and Zeinab Badreddine's PhD) or more general optimal control costs [64].

Let us sketch an important class of open problems. In collaboration with R. McCann [65], 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 [24] a result of density of

uniquely minimizing costs in the C^0-topology. The results in higher topology should be the subject on some further research.

3.4. 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 [32], [74].

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 [34], 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 3.2.2). Proving convergence of the extremals (solutions of the Pontryagin Maximum Principle) is more intricate. In [20], standard averaging ([32], [74]) 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 [53].)

3.5. Other topics

The above does not cover all the fundamentals underlying our research.

- There is a wealth of techniques in linear control and linear identification that we have not mentioned in section 3.1 and are used in work described in sections 4.4 and 6.7 . Stability analysis of dynamical systems is also present here.
- Stochastic control, or more precisely optimal control with stochastic constraints is covered in section 6.6.1 .
- Analysis and structurally stable properties of Hamiltonian dynamics is the domain section 6.1 is most relevant to.

NECS Project-Team

3. Research Program

3.1. Introduction

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

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

3.2. Distributed estimation and data fusion in network systems

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

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

3.3. Network systems and graph analysis

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

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

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

3.4. Collaborative and distributed network control

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

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

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

3.5. Transportation networks

This is currently the main application domain of the NECS team. Several interesting problems in this area capture many of the generic networks problems 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), new collaborative 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 Project-Team

3. Research Program

3.1. General annihilators

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

OQ1) Does a normal form exist for such annihilators?

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

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

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

3.2. Numerical differentiation

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

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

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

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

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

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

3.3. Model-free control

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

3.4. Applications

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

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

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

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 [89], [93]. 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 [66]. 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 [63], [57] 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 [65]. Through a recent experimental work [98], 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 [94] has recently led to a first experimental realization of a full quantum error correcting code improving the coherence time of quantum information [6]. As shown in Figure 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.

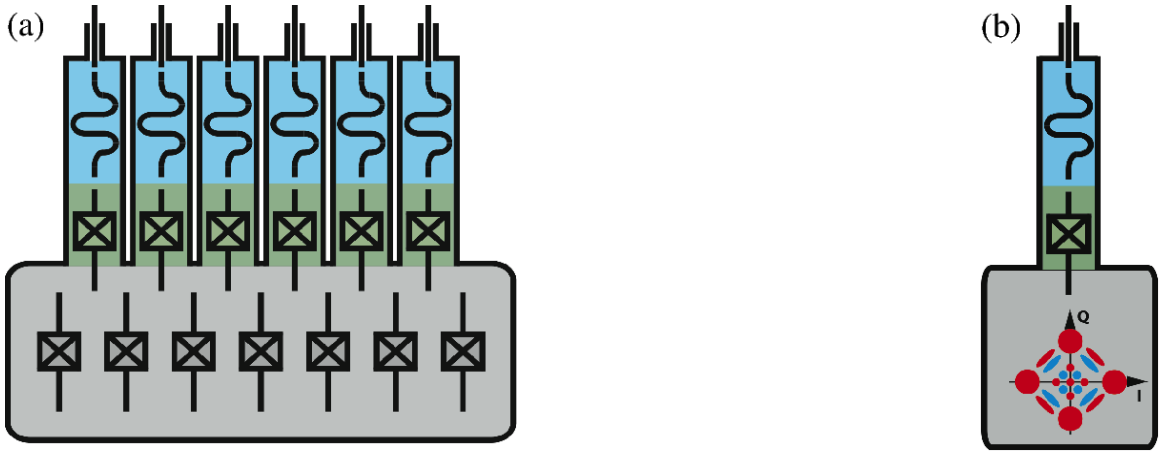

Figure 1. (a) A protected logical qubit consisting of a register of many qubits: here, we see a possible architecture for the Steane code [93] consisting of 7 qubits requiring the measurement of 6 error syndromes. In this sketch, 7 transmon qubits in a high-Q resonator and the measurement of the 6 error 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 the quantum information enabling many-qubit quantum computation or long-distance quantum communication. However, such a closed-loop control which requires a real-time and continuous measurement of the quantum system has been for long considered as counter-intuitive or even impossible. This thought was mainly caused by properties of quantum measurements: any measurement implies an instantaneous strong perturbation to the system's state. The concept of *quantum non-demolotion* (QND) measurement has played a crucial role in understanding and resolving this difficulty [40]. In the context of cavity quantum electro-dynamics (cavity QED) with Rydberg atoms [59], a first experiment on continuous QND measurements of the number of microwave photons was performed by the group at Laboratoire Kastler-Brossel (ENS) [58]. 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 [49], [31], [92], [33]. 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) [48], recent advances in quantum-limited amplifiers [83], [96] have opened doors to high-fidelity non-demolition measurements and real-time feedback for superconducting qubits [60]. 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 [96], [82], [42]. 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 [73].

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 [80] and the closely related coherent feedback [71] 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 [56], single-qubit state stabilization [75], and the creation [35] and stabilization [64], [70][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 [56], [68], [46]. The experimental results based on these protocols have illustrated the efficiency of the approach [56][9]. Through these experiments, we exploit the strong dispersive interaction [87] between superconducting qubits and a single low-Q cavity mode playing the role of a dissipative reservoir. Applying some continuous-wave (cw) microwave drives with well-chosen fixed frequencies, amplitudes, and phases, we engineer an effective interaction Hamiltonian which evacuates entropy from the qubits when an eventual perturbation occurs: by driving the qubits and cavity with continuous-wave drives, we induce an autonomous feedback loop which corrects the state of the qubits every time it decays out of the desired target state. The schemes are robust against small variations of the control parameters (drives amplitudes and phase) and require only some basic calibration. Finally, by avoiding resonant interactions between the qubits and the low-Q cavity mode, the qubits remain protected against the Purcell effect, which would reduce the coherence times. We have also investigated both theoretically and experimentally the autonomous stabilization of non-classical states (such as Schrodinger cat states and Fock states) of microwave field confined in a high-Q cavity mode [74], [85], [61][5].

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 [84], [31], [91], [86], [92], [33][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 [33]: 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 [99]; 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 [78]. 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 [60], [42].

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 [36] and is related to quantum trajectories [44], [47]. A modern and mathematical exposure of the diffusive models is given in [34]. In [100] 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 [84], [91]. This stability result is extended to a large class of continuous-time filters in [32]. Further efforts are required to characterize asymptotic and exponential stability. Estimations of convergence rates are available only for quantum non-demolition measurements [37]. Parameter estimations based on measurement data of quantum trajectories can be formulated within such quantum filtering framework [51], [76].

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 [41] that post-selection statistics and "past quantum" state analysis [52] 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 [80], [71]. 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] [56], 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 [79]). 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., [30][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] [56], [74] 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 [55], [54]. We will start with [88] and [81] where, based on a theorem due to Birkhoff [38], 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 [95] and by our recent generalized extension of the latter synchronizing interactions to quantum systems [72].

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 [77], 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 [97], [69] with experimental limitations. The characterization of Kraus maps to stabilize any types of states has also been established [39], 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 [59], [53]. 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 [67].

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 [43] for the adiabatic elimination of low-Q cavity). Contrarily to the classical composite systems where we have to eliminate one component in a Cartesian product, we here have to eliminate one component in a tensor product. We will adapt geometric singular perturbations [50] and invariant manifold techniques [45] 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 [62] 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 [56][9] [68].

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 [93], [88], [68], 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** ([51], [47], [87], [57], [62], [90], [92], [76], [60]). Many other FSIS have been studied as well. Let us mention [78], [65], [61], [50], [40], [56], [41], [58] 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: [45], [40], [71], [52], [43]). Without approximations, the only known results [48], [49] 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 ([85]). 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 [66], [42], [81].

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 [67] or Kaltenbacher, Neubauer, and Scherzer [69]). 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 [35], [59], [63], [89] for the design of feedback controllers), an input (for instance source inverse problems [32], [44], [53]) 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 ([46]), specific one-dimensional techniques (like in [36]) or observer-based methods as in [73].

   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 [72], 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 [77] or [91]). Using observers, we have proposed in [80], [64] 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 [38], [37].

2. **Geometric inverse problems.**

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

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

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

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

3.3. Numerical analysis and simulation of heterogeneous systems

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

- In the case of FSIS, our main objective is to provide computational tools for the scientific community, essentially to solve academic problems.
- In the case of CWS, our main objective is to build tools general enough to handle industrial problems. Our strong collaboration with Christophe Geuzaine's team in 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. [84], [70], [86], [82], [83], [74]).
- **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) [39], [54], [55] 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 interaction between the incident wave and the scatterers, but also the effects of the interactions between the scatterers themselves. When the number of scatterers is very large (and possibly at high frequency [34], [33]), 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.

TROPICAL Team

3. Research Program

3.1. Optimal control and zero-sum games

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

The geometry of solutions of optimal control and game problems Basic questions include, especially for stationary or ergodic problems, the understanding of existence and uniqueness conditions for the solutions of dynamic programming equations, for instance in terms of controllability or ergodicity properties, and more generally the understanding of the structure of the full set of solutions of stationary Hamilton–Jacobi PDEs and of the set of optimal strategies. These issues are already challenging in the one-player deterministic case, which is an application of choice of tropical methods, since the Lax-Oleinik semigroup, i.e., the evolution semigroup of the Hamilton-Jacobi PDE, is a linear operator in the tropical sense. Recent progress in the deterministic case has been made by combining dynamical systems and PDE techniques (weak KAM theory [75]), and also using metric geometry ideas (abstract boundaries can be used to represent the sets of solutions [89], [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 [48],[12], [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) [76]. 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" [77]. 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) [96], [80]. This suggests that the complexity of control or games problems may be measured by more subtle quantities that the mere number of states, for instance, by some forms of metric entropy (for example, certain large scale problems have a low complexity owing to the presence of decomposition properties, "highway hierarchies", etc.). A second line of of our research is the development of *combinatorial algorithms*, to solve large scale zero-sum two-player problems with discrete state space. This is related to current open problems in algorithmic game theory. In particular, the existence of polynomial-time algorithms for games with ergodic payment is an open question. See e.g. [5] for a polynomial time average complexity result derived by tropical methods. The two lines of research are related, as the understanding of the geometry of solutions allows to develop better approximation or combinatorial algorithms.

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

Several applications (including population dynamics [9] and discrete event systems [61], [67], [54]) 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 [56], [50], tropical semialgebraic sets [59], 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 [14], 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,

$$e^{-a/\epsilon} + e^{-b/\epsilon} \asymp e^{-\min(a,b)/\epsilon} \ , \qquad e^{-a/\epsilon} \times e^{-b/\epsilon} = e^{-(a+b)/\epsilon} \ , \tag{56}$$

when $\epsilon \to 0^+$. Deformations of this kind have been studied in different contexts: large deviations, zero-temperature limits, Maslov's "dequantization method" [95], non-archimedean valuations, log-limit sets and Viro's patchworking method [117], 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 [82], [85].

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 [53], 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 [59], [58], with the goal to better understand complexity issues in classical semidefinite and semi-algebraic programming.

DOLPHIN Team

3. Research Program

3.1. Hybrid multi-objective optimization methods

The success of metaheuristics is based on their ability to find efficient solutions in a reasonable time [43]. But with very large problems and/or multi-objective problems, efficiency of metaheuristics may be compromised. Hence, in this context it is necessary to integrate metaheuristics in more general schemes in order to develop even more efficient methods. For instance, this can be done by different strategies such as cooperation and parallelization.

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

Population-based methods, such as evolutionary algorithms, are well fitted for multi-objective problems, as they work with a set of solutions [39], [42]. To be convinced one may refer to the list of references on Evolutionary Multi-objective Optimization maintained by Carlos A. Coello [0], which contains more than 5500 references. One of the objectives of the project is to propose advanced search mechanisms for intensification and diversification. These mechanisms have been designed in an adaptive manner, since their effectiveness is related to the landscape of the MOP and to the instance solved.

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

3.1.1. Cooperation of metaheuristics

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

Hybrid metaheuristics have received considerable interest these last years in the field of combinatorial optimization. A wide variety of hybrid approaches have been proposed in the literature and give very good results on numerous single objective optimization problems, which are either academic (traveling salesman problem, quadratic assignment problem, scheduling problem, etc) or real-world problems. This efficiency is generally due to the combinations of single-solution based methods (iterative local search, simulated annealing, tabu search, etc) with population-based methods (genetic algorithms, ants search, scatter search, etc). A taxonomy of hybridization mechanisms may be found in [45]. It proposes to decompose these mechanisms into four classes:

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

[0] http://delta.cs.cinvestav.mx/~ccoello/EMOO/EMOObib.html

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

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

3.1.2. Cooperation between metaheuristics and exact methods

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

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

Moreover, a part of the DOLPHIN project deals with studying exact methods in the multi-objective context in order: i) to be able to solve small size problems and to validate proposed heuristic approaches; ii) to have more efficient/dedicated exact methods that can be hybridized with metaheuristics. In this context, the use of parallelism will push back limits of exact methods, which will be able to explore larger size search spaces [40].

3.1.3. Goals

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

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

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

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

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

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

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

3.2.1. Parallel models

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

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

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

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

As these models have now been identified, our objective is to study them in the multi-objective context in order to use them advisedly. Moreover, these models may be merged to combine different levels of parallelism and to obtain more efficient methods [41], [44].

3.2.2. Goals

Our objectives focus on these issues are the following:

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

GEOSTAT Project-Team

3. Research Program

3.1. 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-cale 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 basis), with the aim of finding as less as possible non-zerio 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 ($\gtrsim 0.5$ 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).

GEOSTAT is focusing on the analysis of turbulent datasets in which the multiscale description can be understood in the form of the multiplicative cascade or, in the case of physiological times series, as excitable systems (cardiac electrophysiology: study of intermittency phenomena). The methodological tools used in reaching these objectives place GEOSTAT at the forefront of nonlinear signal processing and analysis of complex systems. We cite: singularity exponents [56], [7] [11], *sparse representations* with reconstruction formulae [13] [57], [5], super-resolution in Oceanography and Earth Observation [10], [2], comparison with embedding techniques such as the one provided by the classical theorem of Takens [54], [44], the use of Lyapunov exponents [27] [20], how they are related to intermittency, persistence along the scales [6], comparison with other approaches such as sparse representations and compressive sensing [https://hal.inria.fr/tel-01239958], and **the ways that lead to effective numerical and high precision determination of nonlinear characteristics in real signals**. Derived from ideas in Statistical Physics, complex signals and systems are studied in relation to the statistical concepts of information content and most informative subsets. As a result, GEOSTAT aims to provide radically new approaches to the study of signals acquired from different complex systems (their analysis, their classification, the study of their dynamical properties etc.). A common characteristic of these signals, which is related to *universality classes* [48] [49] [45], being the existence of a *multiscale organization* of the systems. For instance, the classical notion of edge or border, which is of multiscale nature, and whose importance is well known in Computer Vision and Image Processing, receives profound and rigorous new definitions, in relation with the more physical notion of transition fronts/singularities and fits adequately to the case of chaotic data. The description is analogous to the modeling of states far from equilibrium. From this formalism we derive methods able to determine geometrically the most informative part in a signal scale by scale, which also defines its global properties and allows for compact representation. It appears that the notion of *transition front* in a signal is much more complex than previously expected and, most importantly, related to multiscale notions encountered in the study of nonlinearity [52]. For instance, we give new insights to the computation of dynamical properties in complex signals, in particular in signals for which the classical tools for analyzing dynamics give poor results (such as, for example, correlation methods or optical flow for determining motion in turbulent datasets).

3.2. 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).

3.2.1. Presentation and objectives

Provide state of the art, cutting-edge tools to intra-cardiac multiscale analysis of the electrical activity of fibrillating hearts ; offer physiological hypotheses likely to account for the new quantitative observations together with quantitative simulations.

3.2.2. Results

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. We show that this is incompatible with the common lore for atrial fibrillation based on so-called circuit reentries. 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. In other words, common mathematical models for fibrillation which insist on the intrinsic chaotic dynamics of excitable cells coupled by elliptic propagators (like diffusion) are immune to multifractal scaling. Within this framework, we have developed a new hypothesis in physiology, backed by a mathematical model of gap junction conductance kinetics, that is capable of yielding correct spectra, all based on otherwise known physiology.

3.2.3. Interpretation

Atrial Fibrillation (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 rate of AF recurrences after an initial ablation procedure treating paroxysmal AF increases with time, necessitating multiple redos, and most patients suffering persistent AF are resistant to treatment. The prevailing electrophysiological concepts describing tachy-arrhythmias are more than a century old. They involve abnormal automaticity and conduction. 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". We have analyzed the complexity of voltage signals recovered with bipolar electrodes in the CS during AF. 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 (Ivanov, et al. Nature 399, 461–465) [42]. 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. Contrary to existing mathematical models based on circuit reentries, a spatio-temporal multifractal intermittent dynamics emerges similar to the one found in the CS, opening a new avenue towards the understanding of AF mechanisms of perpetuation. We have shown that the wavelet-based multifractal analysis of long time series of the local impulse energy recorded in the CS of a patient with chronic AF was able to reveal and quantify the intermittent nature of these signals at low frequency ($f < 2$ Hz). To our knowledge, this research is the first to report on the observation and quantification of such multifractal dynamics of the endocavitary electrical activity during AF which is found more complex than previously suspected. Two main observations can be made: (i) the local impulse energy displays different multifractal properties in the left atrial wall area than in the ligament of Marshall area consistently with different anatomical substrate conditions, and (ii) while recorded along the CS vein, the local impulse energy does not exhibit long-range dependence associated with an underlying multiplicative cascade, or in other words the multifractal distribution of the singularities inferred by the two point magnitude analysis does not display any correlation across scales just like a log-normal "multifractal white noise".

This analysis definitely challenges current knowledge in physical, physiological and clinical fundamentals of AF arrhythmia.

The absence of an underlying cascading process is not such a surprise since underlying the multifractal properties displayed by the local impulse energy at low frequencies ($f <\sim 2$ Hz), there is no clear 3D "fragmentation" process inducing some cascading of energy from large to small time scales and also no obvious 2D "aggregation, coalescence or growth" process bringing energy from small to large time scales. What are the physical and physiological mechanisms that drive the multifractal nature of local impulse energy and give rise to the observed differences according to area is still an open question. Nonetheless, these results already undermine the commonly accepted concepts revolving around circuit reentries, and a fortiori spiral waves, as being basic mechanisms for the onset and perpetuation of AF. The mechanistic "wavelength" criterion indeed conveys the idea that random spatio-temporal dispersion of refractoriness, or more generally of functional properties, leads to random mixing of circuit reentries. The "wavelength" scale adjusts naturally to the typical scale λ of dispersion when it exists $c \times RP \lesssim \lambda$ as would be the case for Gaussian statistics of dispersion. In that case, the statistics of the local impulse energy remains Gaussian throughout scales. On the contrary, to fit our new observations we see that the statistics is not Gaussian and evolves across scales through a log-normal propagation law, which accounts for the intermittency, over the range of a few beat cycles ($\sim 0,6$ s) to several tens (~ 10 s and possibly more), therefore spanning the whole atria. Although the ligament of Marshall area is highly innervated, it is quite unlikely that modulations by the ANS, that affects primarily heart rate, play a significant role in the intermittent dynamics, since the documented three peak frequencies at 0,4 Hz, 0,15 Hz and 0,04 Hz do not show up in our analysis. Furthermore, we have found at least two areas with different multifractal regimes. See figure 1 .

Therefore, our findings raise new challenging questions calling for ongoing efforts to develop physiological heart tissue models that account for the low frequency intermittent nature of local impulse energy. In this spirit, in an ongoing research, we propose a model of gap junction conduction remodeling in a denervated heart that accounts for the observed intermittent dynamics over large time scales, as resulting from incoherent random back scatterings, leading to the desynchronization of the network of cardiac excitable cells.

These results have been accepted in a Frontiers in Physiology paper to be published in 2018 https://hal.inria.fr/hal-01673364.

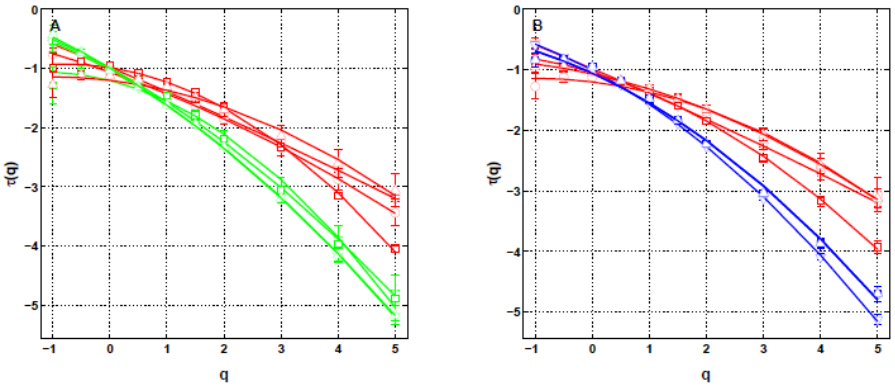

Figure 1. $\tau(q)$ spectra of local impulse energy time-series recorded along the CS vein at the electrodes Pt2 (red), Pt3 (blue) and Pt5 (green). The curves represent quadratic polynomial fit of the data. (A) The symbols correspond to the reference Patient 1 (chronic AF,$\bigtriangledown$), and to 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.

3.3. Multiscale description in terms of multiplicative cascade

GEOSTAT is studying complex signals under the point of view of methods developed in *statistical physics* to study complex systems, with a strong emphasis on multiresolution analysis. Linear methods in signal processing refer to the standard point of view under which operators are expressed by simple convolutions with impulse responses. Linear methods in signal processing are widely used, from least-square deconvolution methods in adaptive optics to source-filter models in speech processing. Because of the absence of localization of the Fourier transform, linear methods are not successful to unlock the multiscale structures and cascading properties of variables which are of primary importance as stated by the physics of the phenomena. This is the reason why new approaches, such as DFA (Detrented Fluctuation Analysis), Time-frequency analysis, variations on curvelets [53] 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 [38], [26], [58], [47]. Some quantities related to nonlinearity, such as Lyapunov exponents, Kolmogorov-Sinai entropy etc. can be computed at least in the phase space [27]. 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 [54] about strange attractors in transition turbulence has motivated the determination of discrete dynamical systems associated to time series [44], and consequently the theoretical determination of nonlinear characteristics associated to complex acquisitions. Emergence phenomena can also be traced inside complex signals themselves, by trying to localize information content geometrically. Fundamentally, in the nonlinear analysis of complex signals there are broadly two approaches: characterization by attractors (embedding and bifurcation) and time-frequency, multiscale/multiresolution approaches. Time-frequency analysis [37] and multiscale/multiresolution are the subjects of intense research and are profoundly reshaping the analysis of complex signals by nonlinear approaches [25], [41]. In real situations, the phase space associated to the acquisition of a complex phenomenon is unknown. It is however possible to relate, inside the signal's domain, local predictability to local reconstruction and deduce from that singularity exponents [11] [7]. We are working on:

- the determination of quantities related to universality classses,
- the geometric localization of multiscale properties in complex signals,
- cascading characteristics of physical variables.

The alternative approach taken in GEOSTAT is microscopical, or geometrical: the multiscale structures which have their "fingerprint" in complex signals are being isolated in a single realization of the complex system, i.e. using the data of the signal itself, as opposed to the consideration of grand ensembles or a wide set of realizations. This is much harder than the ergodic approaches, but it is possible because a reconstruction formula such as the one derived in [55] is local and reconstruction in the signal's domain is related to predictability. This approach is analogous to the consideration of "microcanonical ensembles" in statistical mechanics.

A multiscale organization is a fundamental feature of a complex system, it can be for example related to the cascading properties in turbulent systems. We make use of this kind of description when analyzing turbulent signals: intermittency is observed within the inertial range and is related to the fact that, in the case of FDT,

symmetry is restored only in a statistical sense, a fact that has consequences on the quality of any nonlinear signal representation by frames or dictionaries.

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

The singularity exponents belong to a universality class, independently of microscopic properties in the phase space of various complex systems, and beyond the particular case of turbulent data (where the existence of a multiscale hierarchy, of multifractal nature, can be inferred directly from physical considerations). They describe common multiscale statistical organizations in different complex systems [52], and this is why GEOSTAT is working on nonlinear signal processing tools that are applied to very different types of signals.

For example we give some insight about the collaboration with LEGOS Dynbio team [0] about high-resolution ocean dynamics from microcanonical formulations in nonlinear complex signal analysis. Indeed, synoptic determination of ocean circulation using data acquired from space, with a coherent depiction of its turbulent characteristics remains a fundamental challenge in oceanography. This determination has the potential of revealing all aspects of the ocean dynamic variability on a wide range of spatio-temporal scales and will enhance our understanding of ocean-atmosphere exchanges at super resolution, as required in the present context of climate change. We show that the determination of a multiresolution analysis associated to the multiplicative cascade of a typical physical variable like the Sea Surface Temperature permits an *optimal inference* of oceanic motion field across the scales, resulting in a new method for deriving super resolution oceanic motion from lower resolution altimetry data; the resulting oceanic motion field is validated at super resolution with the use of Lagrangian buoy data available from the Global Drifter Program [0]. In FDT, singularity exponents range in a bounded interval: $]h_\infty, h_{\max}[$ with $h_\infty < 0$ being the most singular exponent. Points $\mathbf{r}$ for which $h(\mathbf{r}) < 0$ localize the strongest transition fronts in the turbulent fluid, where an intensive physical variable like sea surface temperature behaves like $1/\mathbf{r}^{|h(\mathbf{r})|}$. The links between the geometricaly localized singularity exponents, the scaling exponents of structure functions, the multiplicative cascade and the multiscale hierarchy $\mathcal{F}_h$ is the following:

$$\left\{\begin{array}{l} \mathcal{F}_h = \{\mathbf{r} \;\mid\; h(\mathbf{r}) = h\} \\ D(h) = \dim \mathcal{F}_h \\ \tau_p = \inf\limits_h \{ph + 3 - D(h)\} \\ D(h) = \inf\limits_p \{ph + 3 - \tau_p\} \end{array}\right. \tag{57}$$

[0] http://www.legos.obs-mip.fr/recherches/equipes/dynbio.
[0] http://www.aoml.noaa.gov/phod/dac/index.php.

Let $\mathfrak{S}(\mathbf{x})$ be the bidimensionnal signal recording, for each sample point $\mathbf{x}$ representing a pixel on the surface of the ocean of given resolution, the sea surface temperature (sst). To this signal we associate a measure μ whose density w.r.t Lebesgue measure is the signal's gradient norm, and from which the singularity exponents are computed [6]. It is fundamental to notice here that, contrary to other types of exponents computed in Oceanography, such as Finite Size Lyapunov exponents, singularity exponents are computed at instantaneous time, and do not need time series.

Having computed the singularity exponents at each point of a SST signal, a microcanonical version of the multiplicative cascade associated to the scaling properties of the sst becomes available. The idea of the existence of a geometrically localized multiplicative cascade goes back to [51]. The multiplicative cascade, written pointwise, introduces random variables $\eta_{l'/l}(\mathbf{x})$ for $0 < l' < l$ such that

$$\mathcal{T}_\psi \mu(\mathbf{x}, l') \;=\; \eta_{l'/l}(\mathbf{x}) \mathcal{T}_\psi \mu(\mathbf{x}, l) \tag{58}$$

in which the equality is valid pointwise and not only in distribution. Inference of physical variables across the scales is optimized and consequently we describe the multiplicative cascade at each point $\mathbf{x}$ in the signal domain. The injection variables $\eta_{l'/l}(\mathbf{x})$ are indefinitely divisible: $\eta_k(\mathbf{x})\eta_{k'}(\mathbf{x}) \doteq \eta_{kk'}(\mathbf{x})$. It is possible to optimize cross-scale inference of physical variables by considering a *multiresolution analysis* associated to a discrete covering of the "space-frequency" domain. Denoting as usual $(V_j)_{j\in\mathbb{Z}}$ and $(W_j)_{j\in\mathbb{Z}}$ the discrete sequence of approximation and detail spaces associated to a given scaling function, and denoting by $\psi \in L^2(\mathbb{R}^2)$ a wavelet which generates an Hilbertian basis on each detail space W_j, it is known that the detail spaces encode borders and transition information, which is ideally described in the case of turbulent signals by the singularity exponents $\mathbf{h}(\mathbf{x})$. Consequently, a novel idea for super-resolution consists in computing a multiresolution analysis on the signal of singularity exponents $\mathbf{h}(\mathbf{x})$, and to consider that the detail information coming from spaces W_j is given the signal $\mathbf{h}(\mathbf{x})$. The associated orthogonal projection $\pi_j : L^2(\mathbb{R}^2) \to W_j$ defined by $\pi_j(\mathbf{h}) = \sum_{n\in\mathbb{Z}} \langle\, \mathbf{h} \mid \psi_{j,n} \,\rangle \psi_{j,n}$ is then used in the reconstruction formula for retrieving a physical variable at higher resolution from its low resolution counterpart. If $\mathfrak{S}(\mathbf{x})$ is such a variable, we use a reconstruction formula: $A_{j-1}\mathfrak{S} = A_j\mathfrak{S} + \pi_j(\mathbf{h})$ with $A_j : L^2(\mathbb{R}^2) \to V_j$ is the orthogonal projection on the space V_j (approximation operator) and π_j is the orthogonal projection on the detail spaces W_j associated to the signal of singularity exponents $\mathbf{h}(\mathbf{x})$. Validation is performed using Lagrangian buoy data with very good results [10]. We have realized a demonstration movie showing the turbulent ocean dynamics at an SST resolution of 4 km computed from the SST microcanonical cascade and the low-resolution GEKCO product for the year 2006 over the southwestern part of the Indian Ocean. We replace the missing data in the SST MODIS product (clouds and satellite swath) by the corresponding data available from the Operational SST and Sea Ice Analysis (OSTIA) provided by the Group for High-Resolution SST Project [11], which, however, is of lower quality. Two images per day are generated for the whole year of 2006. The resulting images show the norm of the vector field in the background rendered using the line integral convolution algorithm. In the foreground, we show the resulting vector field in a linear gray-scale color map. See link to movie (size: 800 Mo).

3.4. 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 [36], 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 [40], 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 [31], ε-entropy [30]). Complexity measures quantify the presence of structures in the signal (e.g. statistical complexity [33], MPR [46] and others [35]). With these notions, it is already possible to discriminate between random fluctuations and hidden order, such as in chaotic systems [32], [46]. The theory of how information and structures can be defined through scales is not complete yet, but the state of art is promising [34]. 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 [29].

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 [33]. 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 [50]. Recent extensions with advanced clustering techniques [28], [39], 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 [43]. 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

Our research in speech processing focus on the development of novel nonlinear analysis methods for the characterization and classification of pathological and affective speech. For the latter, classical linear methods do not generally capture the nonlinearity, aperiodicity, turbulence and noise that can be present in pathological voices. We thus aim to design and extract new features that allow better characterization/classification of such voices, while being easy to interpret by clinicians. For the former, recent research have shown that the voice source signal information allow significant improvement of speech emotion detection systems. Our goal is to develop novel nonlinear techniques to extract relevant voice source features and to design efficient machine learning algorithms for robust emotion classification.

INOCS Team

3. Research Program

3.1. Introduction

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

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

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

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

3.2. Modeling problems with complex structures

A classical optimization problem can be formulated as follows:

$$\begin{array}{ll} \min & f(x) \\ s.t. & x \in X. \end{array} \tag{59}$$

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:

$$\begin{array}{ll} \min & g(x,y) \\ s.t. & x \in X, \\ (x,y) & \in XY, \\ y & \in Y(x). \end{array} \tag{60}$$

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, Aina Frau Pascual, Stéphane Girard, Julyan Arbel, Gildas Mazo, Jean-Michel Bécu, Hongliang Lu, Emeline Perthame, Fabien Boux, Veronica Munoz Ramirez.

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,

$$f(y_i; \theta) = \sum_{k=1}^{K} P(z_i = k; \theta) f(y_i \mid z_i; \theta) \ . \tag{61}$$

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, Pierre-Antoine Rodesch, Julyan Arbel.

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, Emeline Perthame, Jean-Michel Bécu.

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 [67]. 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 [69] which combines non-parametric regression techniques with parametric dimension reduction aspects. This is also the case in *extreme value analysis* [66], 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).

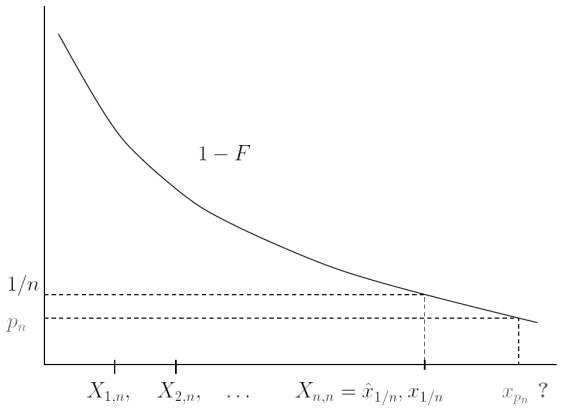

Figure 1. The curve represents the survival function $x \to P(X > x)$. The $1/n$-quantile is estimated by the maximum observation so that $\widehat{x}_{1/n} = X_{n,n}$. As illustrated in the figure, to estimate p_n-quantiles with $p_n < 1/n$, it is necessary to extrapolate beyond the maximum observation.

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:

$$P(X > x) = x^{-1/\theta}\ell(x),\ x > x_0 > 0, \tag{62}$$

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

$$\frac{\ell(tx)}{\ell(x)} \to 1 \text{ as } x \to \infty \tag{63}$$

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:

$$P(X > x) = \exp\{-x^{\theta}\ell(x)\},\ x > x_0 > 0. \tag{64}$$

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

3.3.2. Level sets estimation

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

3.3.3. Dimension reduction

Our work on high dimensional data requires that we face the curse of dimensionality phenomenon. Indeed, the modelling of high dimensional data requires complex models and thus the estimation of high number of parameters compared to the sample size. In this framework, dimension reduction methods aim at replacing the original variables by a small number of linear combinations with as small as a possible loss of information. Principal Component Analysis (PCA) is the most widely used method to reduce dimension in data. However, standard linear PCA can be quite inefficient on image data where even simple image distorsions can lead to highly non-linear data. Two directions are investigated. First, non-linear PCAs can be proposed, leading to semi-parametric dimension reduction methods [68]. 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 [65]. 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 [69].

MODAL Project-Team

3. Research Program

3.1. Generative model design

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

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

3.2. Data visualization

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

RANDOPT Team

3. Research Program

3.1. Developing Novel Theoretical Frameworks for Analyzing and Designing Adaptive Stochastic Algorithms

The lines of research of the RandOpt team are organized along four axis namely developing novel theoretical framework, developing novel algorithms, setting novel standards in scientific experimentation and benchmarking and applications.

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: not only derivatives (gradients) are not exploited, but often the methods are so-called comparison-based which means that the algorithm will only rely on the ranking of the candidate solutions' function values. This renders those methods more robust as they are invariant to strictly increasing transformations of the objective function but at the same time the theoretical analysis becomes more difficult as **we cannot exploit a well defined framework using (strong) properties of the function like convexity or smoothness**.

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, the **critical points of the ODEs are at the boundary of the domain**.

Last, since we aim at developing theory that one 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 to not 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 to analyze one of the core properties of adaptive stochastic methods, namely **linear convergence** on the widest possible class of functions.

We are planning on approaching 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 [15]. 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 [26], 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 [16], [17], [24]. 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. 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.

3.2. Developing Novel Adaptive Stochastic Algorithms

We are planning on developing novel algorithms in the subdomains with strong practical demand for better methods of constrained, multiobjective, large-scale and expensive optimization.

3.2.1. 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 [18]. However, the penalization coefficient is a sensitive parameter that needs to be adapted in order to achieve a robust and general method [19]. 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 [19]. Also, it is particularly only recently that it was pointed out that **linear convergence properties should be preserved** when addressing constraint problems [13].

Promising approaches though, rely on using augmented Lagrangians [13], [14]. 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.

3.2.2. 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. 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 [12], [11]. Yet there are still open problems related to being able to learn both short and long axes in the models.

Another direction, we want to pursue, is exploring the use of large-scale variants of CMA-ES to solve reinforcement learning problems [27].

Last, we are interested to investigate the very-large-scale setting. One approach consist in doing optimization in subspaces. This entails the efficient identification of relevant spaces and the restriction of the optimization to those subspaces.

3.2.3. 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.

3.2.4. 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.

[0] Often, this set forms a manifold of dimension one smaller than the number of objectives.

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.

3.3. 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 [22].

In the RandOpt team we aim at raising the standards for both scientific experimentation and benchmarking.

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 (see also the software section below) 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

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* [76]. 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 [7], [9], [8]. 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 behaviour of unknown data. There is an analogy to game theory where one considers an oblivious adversary choosing the realization that harms the solution the most. A full worst case protection against uncertainty is too conservative and induces very high over-cost. Instead, the realization of random data are bound to belong to a restricted feasibility set, the so-called uncertainty set. Stochastic and robust optimization rely on very large scale programs where probabilistic scenarios are enumerated. There is hope of a tractable solution for realistic size problems, provided one develops very efficient ad-hoc algorithms. The techniques for dynamically handling variables and constraints (column-and-row generation and Bender's projection tools) that are at the core of our team methodological work are specially well-suited to this context.

3.6. Polyhedral Combinatorics and Graph Theory

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

SELECT Project-Team

3. Research Program

3.1. General presentation

From applications we treat on a day-to-day basis, we have learned that some assumptions currently used in asymptotic theory for model selection are often irrelevant in practice. For instance, it is not realistic to assume that the target belongs to the family of models in competition. Moreover, in many situations, it is useful to make the size of the model depend on the sample size, which makes asymptotic analyses breakdown. An important aim of SELECT is to propose model selection criteria which take such practical constraints into account.

3.2. A nonasymptotic view of model selection

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

3.3. Taking into account the modeling purpose in model selection

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

3.4. Bayesian model selection

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

SEQUEL Project-Team

3. Research Program

3.1. In Short

SEQUEL is primarily grounded on two domains:

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

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

3.2. Decision-making Under Uncertainty

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

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

3.2.1. Reinforcement Learning

Sequential decision processes occupy the heart of the SEQUEL project; a detailed presentation of this problem may be found in Puterman's book [69].

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:

$$V^\pi(x) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t | x_0 = x, \pi\right], \tag{65}$$

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 [68]) 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) [66], 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 [67]. 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 $x \in \mathcal{X}$,

$$V^*(x) = \max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V^*(x')\right]. \tag{66}$$

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:

$$\pi^*(x) \in \arg\max_{a \in \mathcal{A}} \sum_{x' \in \mathcal{X}} p(x'|x,a)\left[r(x,a,x') + \gamma V^*(x')\right]. \tag{67}$$

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 ([72]):

- 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 [70], 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.* [65] introduced the algorithm UCB (Upper Confidence Bounds) that follows what is now called the "optimism in the face of uncertainty principle". Their algorithm works by computing upper confidence bounds for all the arms and then choosing the arm with the highest such bound. They proved that the expected regret of their algorithm increases at most

at a logarithmic rate with the number of trials, and that the algorithm achieves the smallest possible regret up to some sub-logarithmic factor (for the considered family of distributions).

3.3. Statistical analysis of time series

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

3.3.1. Prediction of Sequences of Structured and Unstructured Data

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

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

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

3.3.2. Hypothesis testing

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

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

3.3.3. Change Point Analysis

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

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

3.3.4. Clustering Time Series, Online and Offline

The problem of clustering, while being a classical problem of mathematical statistics, belongs to the realm of unsupervised learning. For time series, this problem can be formulated as follows: given several samples $x^1 = (x^1_1, \cdots, x^1_{n_1}), \cdots, x^N = (x^1_N, \cdots, x^N_{n_N})$, 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. Causal modelling

Data science is viewed as an information processing cycle: i) exploiting data and prior knowledge to build models; ii) using models to support optimal decisions in view of desirable ends; and iii) acquiring more data in order to refine the models and/or the desirable ends. Inasmuch data science supports prescriptive recommendations, it requires building causal models: these hold in front of interventions on the application domain − as opposed to predictive models. Causal modelling, acknowledged a priority at the international level (DARPA 2015), opens principled and sound ways to deal with the unbounded expectations / irrational exuberance about Big Data. Furthermore, causality offers an operational framework to better handle transfer learning, semi-supervised learning and missing data.

Mainstream approaches to causality involve restrictive assumptions (no confounders; no causal cycles) with severe scalability limitations [83]. The international challenges proposed by I. Guyon in the last 3 years (See book in preparation) opened brand new research directions, based on learned causation models [78], [75]. The validation of causal graphs still is an open problem in the general case (multiple hypothesis testing issues, heterogeneous variables, temporal dimensions).

TAU is one of the first teams worldwide with expertise in this domain, collaborating with Max Planck Institute (B. Schölkopf), FORTH (I. Tsamardinos) and Facebook Research (D. Lopez Paz). Among the applications calling for causal models are Energy Management (RTE use-cases include failures of equipment and catastrophic cascades of failures; Inria post-doc work of Berna Batu, see Section 4.1) and computational social sciences (with impact on strategic societal issues, see Section 4.2).

3.2. Deep learning

Deep Learning is at the root of quite a few breakthroughs in machine learning and sequential decision making, albeit requiring gigantic resources [72]. Some reasons for these performance jumps are clear (more data, more computational power, more complex search space). Still, the nature of the dynamical system made of training a deep NN yet remains an open question, at the crossroad of information geometry and non-convex optimization. A related open question concerns the neural architecture design. Deep Learning recent developments regarding generative adversarial networks [68] and domain adaptation [67] are relevant to optimal design applications.

The challenges addressed by TAU range from theoretical ML issues (characterization of learnable problems w.r.t the ratio of the data size/neural architecture size) to functional issues (how to encode information invariance and deal with higher order logic beyond convolutional architectures) to societal issues (how to open the black-box of a deep NN and ensure the fairness of the process).

The TAU team has a unique international expertise in three aspects relevant to deep learning, respectively regarding Riemannian geometry [76], [77] (in order to efficiently navigate in the search manifold), statistical physics [66] (to apprehend the learnability region as the architecture size goes to infinity with the data size), and Genetic Programming [57] and neuro-evolution (that provide original avenues for DNN architecture learning). Related industrial contracts involve ADAMME (FUI 2016) and RTE (Energy Management).

3.3. Optimization and Meta-optimization

TAO, with a first-rank expertise worldwide in stochastic black-box optimization, has now been splitted into the new team RANDOPT, and the present team TAU. While RANDOPT further investigates single- and multi-objective continuous stochastic optimization, TAU continues to focus on the fruitful hybridization of ML and stochastic optimization, with the dual persepectives of using ML for a better informed Optimization, and using Optimization to improve ML performances.

One long-term research perspective in the former context is to apprehend the black-box optimization process (BBO) as a sequential optimal decision process, along the lines of the learning to learn framework [58]. An effective policy (in expectation) can be trained on a representative set of benchmark problems, noting that comparison-based BBO methods offer good generalization properties thanks to their invariances properties, opening the road to Riemanian geometric approaches [11]. Another research perspective concerns interactive optimization, where the initially unknown optimization objective is gradually estimated based on the feedback of the human in the loop, and tackled [62], [56]. But this requires making a trade-off between the optimization search space (rich enough to contain good solutions) and the preference search space (simple enough to support effective preference learning with a limited number of queries).
On the other hand, the meta-optimization problem, concerned with selecting a nearly optimal algorithm and its hyper-parameters depending on the problem instance at hand, has been identified a key issue in both ML [61], [59], and Optimization [71]. This issue becomes a bottleneck for the tranfer to industry, due to the acknowledged shortage of data scientists and the increasing complexity of ML/Optimization toolboxes. The *a priori* algorithm selection and calibration in ML is hindered by the lack of appropriate meta-features to describe a problem instance [10], and the state of the art thus relies on Bayesian optimization, alternatively building a surrogate model of algorithm performances on the instance at hand [82]. The search for meta-features can be revisited, exploiting latent representations derived from Collaborative Filtering [10] and Domain Adaptation approaches based on adversarial networks [68], [67].
Note that Isabelle Guyon was the main organizer of the AutoML challenge, whose purpose was to come up with automatic use of ML methods.

3.4. Big Data-Driven Design

Big data-driven modelling/assimilation/simulation/design (BD3) is concerned with the calibration and extension of first principle-based models and equations using data (aka data assimilation), and using such models for optimal design. BD3 can significantly decrease time-to-design, through fast interactions between the modelling, predicting, optimizing, controlling and designing stages, sharing their advances (in particular, coupling first principles and data [63], or repairing/extending closed-form models). Besides the predictive modelling aspects, TAU more specifically investigates the generative and adversarial modelling aspects [68], aimed at data assimilation from biased data.

A first challenge is to find an operational umbrella to handle noisy, sparse, unstructured, missing data, possibly issued from different distributions (e.g. simulated vs real-world data). Collaborative filtering, deep learning, and their hybrids can be used to forge scalable unified intermediate representations, with applications in energy and computational social sciences (involving times series, documents, and/or graphs). Related issues regard the interpretation of such latent representations and the decisions based thereupon. Another challenge is to deliver guarantees for the data-driven models and designs. As more intelligence is put in the modelling, more intelligence must be put in the validation, as reminded by Leon Bottou. Along this way, generative models will be used to support the design of "what if" scenarios, to enhance anomaly detection and monitoring via refined likelihood criteria.

Several recent, on-going, or submitted projects witness the links of TAU members with experts from application domains: in High Energy Physics (LAL, CERN), in space weather (CWI), in anomaly detection (Thalès ThereSIS), and, within the ADAMME project (FUI 2016), in automatic image labelling (Armadillo), and in yield management (VoyagesSncf.com Technologies).

3.5. Transverse Activity: Organisation of Challenges

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 [69], to AutoML [70]. The Higgs challenge [55], most attended ever Kaggle challenge, was jointly organized by TAO (C. Germain), LAL-IN2P3 (B. Kegl) and I. Guyon (not yet at TAO), in collaboration with CERN and Imperial College. The challenge activity continue d within TAU, in relation with fundamental and applied issues.

TAU is particularly implicated with the ChaLearn Looking At People (LAP) challenge series in computer vision, in collaboration with the University of Barcelona [46]. Notably in 2017, TAU co-organized several international LaP challenges:

- ChaLearn Looking at People (LAP) - Job Candidate Screening Coopetition [21]. In conjunction with IJCNN 2017 workshop on explainability in machine learning.
- ChaLearn LAP Real Versus Fake Expressed Emotion Challenge (ICCV 2017) [30].
- ChaLearn LAP Large-scale Continuous Gesture Recognition Challenge (ICCV 2017) [30].
- ChaLearn LAP Large-scale Isolated Gesture Recognition Challenge (ICCV 2017) [30].

TAU was also implicated in organizing a follow up of the AutoML challenge for the PAKDD conference. TAU also co-organized local events (hackathons), as "rehearsals" of international competitions in preparation:

- Spatio-temporal time series challenges for the European See.4C challenge about Energy Management (Paris, 14/2/2017, and Toulon, 22/4/2017). Book with Sprimger in preparation.
- Track ML: tracking particles in high energy physics (Orsay, 21/3/2017) [16].

The Codalab challenge platform, originally designed within Microsoft Research with Isabelle Guyon as one of the PIs, has now been migrated to U. Paris-Sud. It is an open source project. Part of the development is supported by Isabelle Guyon's Paris-Saclay chair (co-funded by Inria). Codalab's user base has been steadily growing. At the end of 2017, we now have over 10'000 users who have entered more than 480 challenges (145 of which are public).

This year, there was a major upgrade of Codalab, featuring:

- A step-by-step Wizard to guide beginner challenge organizers through the process of organizing challenges. This Wizard facilitates the work of students learning to organize challenges.
- Use of dockers and queues, allowing challenge participants to easily use their own computer resources in the backend to support challenges with code submissions.
- A modular competition logic, which will enable supporting new types of challenges such as reinforcement learning competitions.

ASPI Team

3. Research Program

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

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

A major breakthrough made in the mid 90's, has been the introduction of interacting Monte Carlo methods, also known as sequential Monte Carlo (SMC) methods, in which a whole (possibly weighted) sample, called *system of particles*, is propagated in time, where the particles

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

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

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

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

In the special case of particle filtering, originally developed within the tracking community, the algorithms yield a numerical approximation of the optimal Bayesian filter, i.e. of the conditional probability distribution of the hidden state given the past observations, as a (possibly weighted) empirical probability distribution of the system of particles. In its simplest version, introduced in several different scientific communities under the name of *bootstrap filter* [38], *Monte Carlo filter* [43] or *condensation* (conditional density propagation) algorithm [42], and which historically has been the first algorithm to include a resampling step, the selection mechanism is governed by the likelihood function: at each time step, a particle is more likely to survive and to replicate at the next generation if it is consistent with the current observation. The algorithms also provide as a by–product a numerical approximation of the likelihood function, and of many other contrast functions for parameter estimation in hidden Markov models, such as the prediction error or the conditional least–squares criterion.

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

> positioning, navigation, and tracking [39], [32], visual tracking [42], mobile robotics [33], [55], ubiquitous computing and ambient intelligence, sensor networks, risk evaluation and simulation of rare events [37], genetics, molecular simulation [34], etc.

Other examples of the many applications of particle filtering can be found in the contributed volume [22] and in the special issue of *IEEE Transactions on Signal Processing* devoted to *Monte Carlo Methods for Statistical Signal Processing* in February 2002, where the tutorial paper [23] can be found, and in the textbook [51] devoted to applications in target tracking. Applications of sequential Monte Carlo methods to other areas, beyond signal and image processing, e.g. to genetics, can be found in [48]. A recent overview can also be found in [25].

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

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

These algorithms can be interpreted as numerical approximation schemes for Feynman–Kac distributions, a pathwise generalization of Gibbs–Boltzmann distributions, in terms of the weighted empirical probability distribution associated with a system of particles. This abstract point of view [30], [29], has proved to be extremely fruitful in providing a very general framework to the design and analysis of numerical approximation schemes, based on systems of branching and / or interacting particles, for nonlinear dynamical systems with values in the space of probability distributions, associated with Feynman–Kac distributions. Many asymptotic results have been proved as the number N of particles (sample size) goes to infinity, using techniques coming from applied probability (interacting particle systems, empirical processes [58]), see e.g. the survey article [30] or the textbooks [29], [28], and references therein

> convergence in $\mathbb{L}^p$, convergence as empirical processes indexed by classes of functions, uniform convergence in time, see also [46], [47], central limit theorem, see also [44], [31], propagation of chaos, large deviations principle, etc.

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

3.2. Multilevel splitting for rare event simulation

See 4.2 , 5.1 , and 5.2 .

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

> nuclear power plants, food industry, telecommunication networks, finance and insurance industry, air traffic management, etc.

In such complex systems, analytical methods cannot be used, and naive Monte Carlo methods are clearly unefficient to estimate accurately very small probabilities. Besides importance sampling, an alternate widespread technique consists in multilevel splitting [45], where trajectories going towards the critical set are given offsprings, thus increasing the number of trajectories that eventually reach the critical set. As shown in [6], the Feynman–Kac formalism of 3.1 is well suited for the design and analysis of splitting algorithms for rare event simulation.

Propagation of uncertainty Multilevel splitting can be used in static situations. Here, the objective is to learn the probability distribution of an output random variable $Y = F(X)$, where the function F is only defined pointwise for instance by a computer programme, and where the probability distribution of the input random variable X is known and easy to simulate from. More specifically, the objective could be to compute the probability of the output random variable exceeding a threshold, or more generally to evaluate the cumulative distribution function of the output random variable for different output values. This problem is characterized by the lack of an analytical expression for the function, the computational cost of a single pointwise evaluation of the function, which means that the number of calls to the function should be limited as much as possible, and finally the complexity and / or unavailability of the source code of the computer programme, which makes any modification very difficult or even impossible, for instance to change the model as in importance sampling methods.

The key issue is to learn as fast as possible regions of the input space which contribute most to the computation of the target quantity. The proposed splitting methods consists in (i) introducing a sequence of intermediate regions in the input space, implicitly defined by exceeding an increasing sequence of thresholds or levels, (ii) counting the fraction of samples that reach a level given that the previous level has been reached already, and (iii) improving the diversity of the selected samples, usually with an artificial Markovian dynamics for the input variable. In this way, the algorithm learns

- the transition probability between successive levels, hence the probability of reaching each intermediate level,
- and the probability distribution of the input random variable, conditionned on the output variable reaching each intermediate level.

A further remark, is that this conditional probability distribution is precisely the optimal (zero variance) importance distribution needed to compute the probability of reaching the considered intermediate level.

Rare event simulation To be specific, consider a complex dynamical system modelled as a Markov process, whose state can possibly contain continuous components and finite components (mode, regime, etc.), and the objective is to compute the probability, hopefully very small, that a critical region of the state space is reached by the Markov process before a final time T, which can be deterministic and fixed, or random (for instance the time of return to a recurrent set, corresponding to a nominal behaviour).

The proposed splitting method consists in (i) introducing a decreasing sequence of intermediate, more and more critical, regions in the state space, (ii) counting the fraction of trajectories that reach an intermediate region before time T, given that the previous intermediate region has been reached before time T, and (iii) regenerating the population at each stage, through resampling. In addition to the non–intrusive behaviour of the method, the splitting methods make it possible to learn the probability distribution of typical critical trajectories, which reach the critical region before final time T, an important feature that methods based on importance sampling usually miss. Many variants have been proposed, whether

- the branching rate (number of offsprings allocated to a successful trajectory) is fixed, which allows for depth–first exploration of the branching tree, but raises the issue of controlling the population size,
- the population size is fixed, which requires a breadth–first exploration of the branching tree, with random (multinomial) or deterministic allocation of offsprings, etc.

Just as in the static case, the algorithm learns

- the transition probability between successive levels, hence the probability of reaching each intermediate level,
- and the entrance probability distribution of the Markov process in each intermediate region.

Contributions have been given to

- minimizing the asymptotic variance, obtained through a central limit theorem, with respect to the shape of the intermediate regions (selection of the importance function), to the thresholds (levels), to the population size, etc.

- controlling the probability of extinction (when not even one trajectory reaches the next intermediate level),
- designing and studying variants suited for hybrid state space (resampling per mode, marginalization, mode aggregation),

and in the static case, to

- minimizing the asymptotic variance, obtained through a central limit theorem, with respect to intermediate levels, to the Metropolis kernel introduced in the mutation step, etc.

A related issue is global optimization. Indeed, the difficult problem of finding the set M of global minima of a real–valued function V can be replaced by the apparently simpler problem of sampling a population from a probability distribution depending on a small parameter, and asymptotically supported by the set M as the small parameter goes to zero. The usual approach here is to use the cross–entropy method [52], [27], which relies on learning the optimal importance distribution within a prescribed parametric family. On the other hand, multilevel splitting methods could provide an alternate nonparametric approach to this problem.

3.3. Statistical learning: pattern recognition and nonparametric regression

In pattern recognition and statistical learning, also known as machine learning, nearest neighbor (NN) algorithms are amongst the simplest but also very powerful algorithms available. Basically, given a training set of data, i.e. an N–sample of i.i.d. object–feature pairs, with real–valued features, the question is how to generalize, that is how to guess the feature associated with any new object. To achieve this, one chooses some integer k smaller than N, and takes the mean–value of the k features associated with the k objects that are nearest to the new object, for some given metric.

In general, there is no way to guess exactly the value of the feature associated with the new object, and the minimal error that can be done is that of the Bayes estimator, which cannot be computed by lack of knowledge of the distribution of the object–feature pair, but the Bayes estimator can be useful to characterize the strength of the method. So the best that can be expected is that the NN estimator converges, say when the sample size N grows, to the Bayes estimator. This is what has been proved in great generality by Stone [53] for the mean square convergence, provided that the object is a finite–dimensional random variable, the feature is a square–integrable random variable, and the ratio k/N goes to 0. Nearest neighbor estimator is not the only local averaging estimator with this property, but it is arguably the simplest.

The asymptotic behavior when the sample size grows is well understood in finite dimension, but the situation is radically different in general infinite dimensional spaces, when the objects to be classified are functions, images, etc.

Nearest neighbor classification in infinite dimension In finite dimension, the k–nearest neighbor classifier is universally consistent, i.e. its probability of error converges to the Bayes risk as N goes to infinity, whatever the joint probability distribution of the pair, provided that the ratio k/N goes to zero. Unfortunately, this result is no longer valid in general metric spaces, and the objective is to find out reasonable sufficient conditions for the weak consistency to hold. Even in finite dimension, there are exotic distances such that the nearest neighbor does not even get closer (in the sense of the distance) to the point of interest, and the state space needs to be complete for the metric, which is the first condition. Some regularity on the regression function is required next. Clearly, continuity is too strong because it is not required in finite dimension, and a weaker form of regularity is assumed. The following consistency result has been obtained: if the metric space is separable and if some Besicovich condition holds, then the nearest neighbor classifier is weakly consistent. Note that the Besicovich condition is always fulfilled in finite dimensional vector spaces (this result is called the Besicovich theorem), and that a counterexample [4] can be given in an infinite dimensional space with a Gaussian measure (in this case, the nearest neighbor classifier is clearly nonconsistent). Finally, a simple example has been found which verifies the Besicovich condition with a noncontinuous regression function.

Rates of convergence of the functional k–nearest neighbor estimator Motivated by a broad range of potential applications, such as regression on curves, rates of convergence of the k–nearest neighbor estimator of the regression function, based on N independent copies of the object–feature pair, have been investigated when the object is in a suitable ball in some functional space. Using compact embedding theory, explicit and general finite sample bounds can be obtained for the expected squared difference between the k–nearest neighbor estimator and the Bayes regression function, in a very general setting. The results have also been particularized to classical function spaces such as Sobolev spaces, Besov spaces and reproducing kernel Hilbert spaces. The rates obtained are genuine nonparametric convergence rates, and up to our knowledge the first of their kind for k–nearest neighbor regression.

This topic has produced several theoretical advances [1], [2] in collaboration with Gérard Biau (université Pierre et Marie Curie). A few possible target application domains have been identified in

- the statistical analysis of recommendation systems,
- the design of reduced–order models and analog samplers,

that would be a source of interesting problems.

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 [53] and Duan and Li [51].
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 [52].

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, DCNS 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. Dependence modeling

Participants: Aurélien Alfonsi, Benjamin Jourdain, Damien Lamberton, Bernard Lapeyre.

The volatility is a key concept in modern mathematical finance, and an indicator of the market stability. Risk management and associated instruments depend strongly on the volatility, and volatility modeling has thus become a crucial issue in the finance industry. Of particular importance is the assets *dependence* modeling. The calibration of models for a single asset can now be well managed by banks but modeling of dependence is the bottleneck to efficiently aggregate such models. A typical issue is how to go from the individual evolution of each stock belonging to an index to the joint modeling of these stocks. In this perspective, we want to model stochastic volatility in a *multidimensional* framework. To handle these questions mathematically, we have to deal with stochastic differential equations that are defined on matrices in order to model either the instantaneous covariance or the instantaneous correlation between the assets. From a numerical point of view, such models are very demanding since the main indexes include generally more than thirty assets. It is therefore necessary to develop efficient numerical methods for pricing options and calibrating such models to market data. As a first application, modeling the dependence between assets allows us to better handle derivatives products on a basket. It would give also a way to price and hedge consistensly single-asset and basket products. Besides, it can be a way to capture how the market estimates the dependence between assets. This could give some insights on how the market anticipates the systemic risk.

3.2. Liquidity risk

Participants: Aurélien Alfonsi, Agnès Sulem, Antonino Zanette.

The financial crisis has caused an increased interest in mathematical finance studies which take into account the market incompleteness issue and the liquidity risk. Loosely speaking, liquidity risk is the risk that comes from the difficulty of selling (or buying) an asset. At the extreme, this may be the impossibility to sell an asset, which occurred for "junk assets" during the subprime crisis. Hopefully, it is in general possible to sell assets, but this may have some cost. Let us be more precise. Usually, assets are quoted on a market with a Limit Order Book (LOB) that registers all the waiting limit buy and sell orders for this asset. The bid (resp. ask) price is the most expensive (resp. cheapest) waiting buy or sell order. If a trader wants to sell a single asset, he will sell it at the bid price. Instead, if he wants to sell a large quantity of assets, he will have to sell them at a lower price in order to match further waiting buy orders. This creates an extra cost, and raises important issues. From a short-term perspective (from few minutes to some days), this may be interesting to split the selling order and to focus on finding optimal selling strategies. This requires to model the market microstructure, i.e. how the market reacts in a short time-scale to execution orders. From a long-term perspective (typically, one month or more), one has to understand how this cost modifies portfolio managing strategies (especially delta-hedging or optimal investment strategies). At this time-scale, there is no need to model precisely the market microstructure, but one has to specify how the liquidity costs aggregate.

3.2.1. Long term liquidity risk.

On a long-term perspective, illiquidity can be approached via various ways: transactions costs [46], [47], [53], [58], [61], [73], [70], delay in the execution of the trading orders [74], [72], [55], trading constraints or restriction on the observation times (see e.g. [60] and references herein). As far as derivative products are concerned, one has to understand how delta-hedging strategies have to be modified. This has been considered for example by Cetin, Jarrow and Protter [71]. We plan to contribute on these various aspects of liquidity risk modeling and associated stochastic optimization problems. Let us mention here that the price impact generated by the trades of the investor is often neglected with a long-term perspective. This seems acceptable

since the investor has time enough to trade slowly in order to eliminate its market impact. Instead, when the investor wants to make significant trades on a very short time horizon, it is crucial to take into account and to model how prices are modified by these trades. This question is addressed in the next paragraph on market microstructure.

3.2.2. Market microstructure.

The European directive MIFID has increased the competition between markets (NYSE-Euronext, Nasdaq, LSE and new competitors). As a consequence, the cost of posting buy or sell orders on markets has decreased, which has stimulated the growth of market makers. Market makers are posting simultaneously bid and ask orders on a same stock, and their profit comes from the bid-ask spread. Basically, their strategy is a "round-trip" (i.e. their position is unchanged between the beginning and the end of the day) that has generated a positive cash flow.

These new rules have also greatly stimulated research on market microstructure modeling. From a practitioner point of view, the main issue is to solve the so-called "optimal execution problem": given a deadline T, what is the optimal strategy to buy (or sell) a given amount of shares that achieves the minimal expected cost? For large amounts, it may be optimal to split the order into smaller ones. This is of course a crucial issue for brokers, but also market makers that are looking for the optimal round-trip.

Solving the optimal execution problem is not only an interesting mathematical challenge. It is also a mean to better understand market viability, high frequency arbitrage strategies and consequences of the competition between markets. For example when modeling the market microstructure, one would like to find conditions that allow or exclude round trips. Beyond this, even if round trips are excluded, it can happen that an optimal selling strategy is made with large intermediate buy trades, which is unlikely and may lead to market instability.

We are interested in finding synthetic market models in which we can describe and solve the optimal execution problem. A. Alfonsi and A. Schied (Mannheim University) [48] have already proposed a simple Limit Order Book model (LOB) in which an explicit solution can be found for the optimal execution problem. We are now interested in considering more sophisticated models that take into account realistic features of the market such as short memory or stochastic LOB. This is mid term objective. At a long term perspective one would like to bridge these models to the different agent behaviors, in order to understand the effect of the different quotation mechanisms (transaction costs for limit orders, tick size, etc.) on the market stability.

3.3. Contagion modeling and systemic risk

Participants: Benjamin Jourdain, Agnès Sulem.

After the recent financial crisis, systemic risk has emerged as one of the major research topics in mathematical finance. The scope is to understand and model how the bankruptcy of a bank (or a large company) may or not induce other bankruptcies. By contrast with the traditional approach in risk management, the focus is no longer on modeling the risks faced by a single financial institution, but on modeling the complex interrelations between financial institutions and the mechanisms of distress propagation among these. Ideally, one would like to be able to find capital requirements (such as the one proposed by the Basel committee) that ensure that the probability of multiple defaults is below some level.

The mathematical modeling of default contagion, by which an economic shock causing initial losses and default of a few institutions is amplified due to complex linkages, leading to large scale defaults, can be addressed by various techniques, such as network approaches (see in particular R. Cont et al. [49] and A. Minca [65]) or mean field interaction models (Garnier-Papanicolaou-Yang [59]). The recent approach in [49] seems very promising. It describes the financial network approach as a weighted directed graph, in which nodes represent financial institutions and edges the exposures between them. Distress propagation in a financial system may be modeled as an epidemics on this graph. In the case of incomplete information on the structure of the interbank network, cascade dynamics may be reduced to the evolution of a multi-dimensional Markov chain that corresponds to a sequential discovery of exposures and determines at any time the size of contagion. Little has been done so far on the *control* of such systems in order to reduce the systemic risk and we aim to contribute to this domain.

3.4. Stochastic analysis and numerical probability

3.4.1. Stochastic control

Participants: Vlad Bally, Jean-Philippe Chancelier, Marie-Claire Quenez, Agnès Sulem.

The financial crisis has caused an increased interest in mathematical finance studies which take into account the market incompleteness issue and the default risk modeling, the interplay between information and performance, the model uncertainty and the associated robustness questions, and various nonlinearities. We address these questions by further developing the theory of stochastic control in a broad sense, including stochastic optimization, nonlinear expectations, Malliavin calculus, stochastic differential games and various aspects of optimal stopping.

3.4.2. Optimal stopping

Participants: Aurélien Alfonsi, Benjamin Jourdain, Damien Lamberton, Agnès Sulem, Marie-Claire Quenez.

The theory of American option pricing has been an incite for a number of research articles about optimal stopping. Our recent contributions in this field concern optimal stopping in models with jumps, irregular obstacles, free boundary analysis, reflected BSDEs.

3.4.3. Simulation of stochastic differential equations

Participants: Benjamin Jourdain, Aurélien Alfonsi, Vlad Bally, Damien Lamberton, Bernard Lapeyre, Jérôme Lelong, Céline Labart.

Effective numerical methods are crucial in the pricing and hedging of derivative securities. The need for more complex models leads to stochastic differential equations which cannot be solved explicitly, and the development of discretization techniques is essential in the treatment of these models. The project MathRisk addresses fundamental mathematical questions as well as numerical issues in the following (non exhaustive) list of topics: Multidimensional stochastic differential equations, High order discretization schemes, Singular stochastic differential equations, Backward stochastic differential equations.

3.4.4. Monte-Carlo simulations

Participants: Benjamin Jourdain, Aurélien Alfonsi, Damien Lamberton, Vlad Bally, Bernard Lapeyre, Ahmed Kebaier, Céline Labart, Jérôme Lelong, Antonino Zanette.

Monte-Carlo methods is a very useful tool to evaluate prices especially for complex models or options. We carry on research on *adaptive variance reduction methods* and to use *Monte-Carlo methods for calibration* of advanced models.

This activity in the MathRisk team is strongly related to the development of the Premia software.

3.4.5. Malliavin calculus and applications in finance

Participants: Vlad Bally, Arturo Kohatsu-Higa, Agnès Sulem, Antonino Zanette.

The original Stochastic Calculus of Variations, now called the Malliavin calculus, was developed by Paul Malliavin in 1976 [63]. It was originally designed to study the smoothness of the densities of solutions of stochastic differential equations. One of its striking features is that it provides a probabilistic proof of the celebrated Hörmander theorem, which gives a condition for a partial differential operator to be hypoelliptic. This illustrates the power of this calculus. In the following years a lot of probabilists worked on this topic and the theory was developed further either as analysis on the Wiener space or in a white noise setting. Many applications in the field of stochastic calculus followed. Several monographs and lecture notes (for example D. Nualart [66], D. Bell [52] D. Ocone [68], B. Øksendal [75]) give expositions of the subject. See also V. Bally [50] for an introduction to Malliavin calculus.

From the beginning of the nineties, applications of the Malliavin calculus in finance have appeared : In 1991 Karatzas and Ocone showed how the Malliavin calculus, as further developed by Ocone and others, could be used in the computation of hedging portfolios in complete markets [67].

Since then, the Malliavin calculus has raised increasing interest and subsequently many other applications to finance have been found [64], such as minimal variance hedging and Monte Carlo methods for option pricing. More recently, the Malliavin calculus has also become a useful tool for studying insider trading models and some extended market models driven by Lévy processes or fractional Brownian motion.

We give below an idea why Malliavin calculus may be a useful instrument for probabilistic numerical methods.

We recall that the theory is based on an integration by parts formula of the form $E(f'(X)) = E(f(X)Q)$. Here X is a random variable which is supposed to be "smooth" in a certain sense and non-degenerated. A basic example is to take $X = \sigma\Delta$ where Δ is a standard normally distributed random variable and σ is a strictly positive number. Note that an integration by parts formula may be obtained just by using the usual integration by parts in the presence of the Gaussian density. But we may go further and take X to be an aggregate of Gaussian random variables (think for example of the Euler scheme for a diffusion process) or the limit of such simple functionals.

An important feature is that one has a relatively explicit expression for the weight Q which appears in the integration by parts formula, and this expression is given in terms of some Malliavin-derivative operators.

Let us now look at one of the main consequences of the integration by parts formula. If one considers the *Dirac* function $\delta_x(y)$, then $\delta_x(y) = H'(y-x)$ where H is the *Heaviside* function and the above integration by parts formula reads $E(\delta_x(X)) = E(H(X-x)Q)$, where $E(\delta_x(X))$ can be interpreted as the density of the random variable X. We thus obtain an integral representation of the density of the law of X. This is the starting point of the approach to the density of the law of a diffusion process: the above integral representation allows us to prove that under appropriate hypothesis the density of X is smooth and also to derive upper and lower bounds for it. Concerning simulation by Monte Carlo methods, suppose that you want to compute $E(\delta_x(y)) \sim \frac{1}{M}\sum_{i=1}^{M} \delta_x(X^i)$ where $X^1, ..., X^M$ is a sample of X. As X has a law which is absolutely continuous with respect to the Lebesgue measure, this will fail because no X^i hits exactly x. But if you are able to simulate the weight Q as well (and this is the case in many applications because of the explicit form mentioned above) then you may try to compute $E(\delta_x(X)) = E(H(X-x)Q) \sim \frac{1}{M}\sum_{i=1}^{M} E(H(X^i-x)Q^i)$. This basic remark formula leads to efficient methods to compute by a Monte Carlo method some irregular quantities as derivatives of option prices with respect to some parameters (the *Greeks*) or conditional expectations, which appear in the pricing of American options by the dynamic programming). See the papers by Fournié et al [57] and [56] and the papers by Bally et al., Benhamou, Bermin et al., Bernis et al., Cvitanic et al., Talay and Zheng and Temam in [62].

L. Caramellino, A. Zanette and V. Bally have been concerned with the computation of conditional expectations using Integration by Parts formulas and applications to the numerical computation of the price and the Greeks (sensitivities) of American or Bermudean options. The aim of this research was to extend a paper of Reigner and Lions who treated the problem in dimension one to higher dimension - which represent the real challenge in this field. Significant results have been obtained up to dimension 5 [51] and the corresponding algorithms have been implemented in the Premia software.

Moreover, there is an increasing interest in considering jump components in the financial models, especially motivated by calibration reasons. Algorithms based on the integration by parts formulas have been developed in order to compute Greeks for options with discontinuous payoff (e.g. digital options). Several papers and two theses (M. Messaoud and M. Bavouzet defended in 2006) have been published on this topic and the corresponding algorithms have been implemented in Premia. Malliavin Calculus for jump type diffusions - and more general for random variables with locally smooth law - represents a large field of research, also for applications to credit risk problems.

The Malliavin calculus is also used in models of insider trading. The "enlargement of filtration" technique plays an important role in the modeling of such problems and the Malliavin calculus can be used to obtain general results about when and how such filtration enlargement is possible. See the paper by P. Imkeller in [62]). Moreover, in the case when the additional information of the insider is generated by adding the information about the value of one extra random variable, the Malliavin calculus can be used to find explicitly the optimal

portfolio of an insider for a utility optimization problem with logarithmic utility. See the paper by J.A. León, R. Navarro and D. Nualart in [62]).

A. Kohatsu Higa and A. Sulem have studied a controlled stochastic system whose state is described by a stochastic differential equation with anticipating coefficients. These SDEs can be interpreted in the sense of *forward integrals*, which are the natural generalization of the semi-martingale integrals, as introduced by Russo and Valois [69]. This methodology has been applied for utility maximization with insiders.

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.