RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

Activity Report 2018

Section Application Domains

Edition: 2019-03-07

NUMERICAL SCHEMES AND SIMULATIONS

OPTIMIZATION AND CONTROL OF DYNAMIC SYSTEMS

OPTIMIZATION, MACHINE LEARNING AND STATISTICAL METHODS

STOCHASTIC APPROACHES

ACUMES Project-Team

4. Application Domains

4.1. Active flow control for vehicles

The reduction of CO2 emissions represents a great challenge for the automotive and aeronautic industries, which committed respectively a decrease of 20% for 2020 and 75% for 2050. This goal will not be reachable, unless a significant improvement of the aerodynamic performance of cars and aircrafts is achieved (e.g. aerodynamic resistance represents 70% of energy losses for cars above 90 km/h). Since vehicle design cannot be significantly modified, due to marketing or structural reasons, active flow control technologies are one of the most promising approaches to improve aerodynamic performance. This consists in introducing micro-devices, like pulsating jets or vibrating membranes, that can modify vortices generated by vehicles. Thanks to flow non-linearities, a small energy expense for actuation can significantly reduce energy losses. The efficiency of this approach has been demonstrated, experimentally as well as numerically, for simple configurations [155]. However, the lack of efficient and flexible numerical models, that allow to simulate and optimize a large number of such devices on realistic configurations, is still a bottleneck for the emergence of this technology in an industrial context. In particular, the prediction of actuated flows requires the use of advanced turbulence closures, like Detached Eddy Simulation or Large Eddy Simulation [104]. They are intrinsically three-dimensional and unsteady, yielding a huge computational effort for each analysis, which makes their use tedious for optimization purpose. In this context, we intend to contribute to the following research axes:

- *Sensitivity analysis for actuated flows.* Adjoint-based (reverse) approaches, classically employed in design optimization procedure to compute functional gradients, are not well suited to this context. Therefore, we propose to explore the alternative (direct) formulation, which is not so much used, in the perspective of a better characterization of actuated flows and optimization of control devices.
- *Hierarchical optimization of control devices.* The optimization of dozen of actuators, in terms of locations, frequencies, amplitudes, will be practically tractable only if a hierarchical approach is adopted, which mixes fine (DES) and coarse (URANS) simulations, and possibly experiments. We intend to develop such an optimization strategy on the basis of Gaussian Process models (*multi-fidelity kriging*).

4.2. Vehicular and pedestrian traffic flows

Intelligent Transportation Systems (ITS) is nowadays a booming sector, where the contribution of mathematical modeling and optimization is widely recognized. In this perspective, traffic flow models are a commonly cited example of "complex systems", in which individual behavior and self-organization phenomena must be taken into account to obtain a realistic description of the observed macroscopic dynamics [114]. Further improvements require more advanced models, keeping into better account interactions at the microscopic scale, and adapted control techniques, see [63] and references therein. In particular, we will focus on the following aspects:

- *Junction models.* We are interested in designing a general junction model both satisfying basic analytical properties guaranteeing well-posedness and being realistic for traffic applications. In particular, the model should be able to overcome severe drawbacks of existing models, such as restrictions on the number of involved roads and prescribed split ratios [76], [102], which limit their applicability to real world situations. Hamilton-Jacobi equations could be also an interesting direction of research, following the recent results obtained in [119].
- *Data assimilation.* In traffic flow modeling, the capability of correctly estimating and predicting the state of the system depends on the availability of rich and accurate data on the network. Up to now, the most classical sensors are fixed ones. They are composed of inductive loops (electrical wires) that are installed at different spatial positions of the network and that can measure the traffic flow,

the occupancy rate (i.e. the proportion of time during which a vehicle is detected to be over the loop) and the speed (in case of a system of two distant loops). These data are useful / essential to calibrate the phenomenological relationship between flow and density which is known in the traffic literature as the Fundamental Diagram. Nowadays, thanks to the wide development of mobile internet and geolocalization techniques and its increasing adoption by the road users, smartphones have turned into perfect mobile sensors in many domains, including in traffic flow management. They can provide the research community with a large database of individual trajectory sets that are known as Floating Car Data (FCD), see [116] for a real field experiment. Classical macroscopic models, say (hyperbolic systems of) conservation laws, are not designed to take into account this new kind of microscopic data. Other formulations, like Hamilton-Jacobi partial differential equations, are most suited and have been intensively studied in the past five years (see [69], [70]), with a stress on the (fixed) Eulerian framework. Up to our knowledge, there exist a few studies in the time-Lagrangian as well as space-Lagrangian frameworks, where data coming from mobile sensors could be easily assimilated, due to the fact that the Lagrangian coordinate (say the label of a vehicle) is fixed.

- *Control of autonomous vehicles.* Traffic flow is usually controlled via traffic lights or variable speed limits, which have fixed space locations. The deployment of autonomous vehicles opens new perspectives in traffic management, as the use of a small fraction of cars to optimize the overall traffic. In this perspective, the possibility to track vehicles trajectories either by coupled micro-macro models [84], [103] or via the Hamilton-Jacobi approach [69], [70] could allow to optimize the flow by controlling some specific vehicles corresponding to internal conditions.

4.3. Virtual Fractional Flow Reserve in Coronary stenting

Atherosclerosis is a chronic inflammatory disease that affects the entire arterial network and especially the coronary arteries. It is an accumulation of lipids over the arterial surface due to a dysfunction of this latter. The objective of clinical intervention, in this case, is to establish a revascularization using different angioplasty techniques, among which the implantation of stents is the most widespread. This intervention involves introducing a stent into the damaged portion in order to allow the blood to circulate in a normal way over all the vessels. Revascularization is based on the principle of remedying ischemia, which is a decrease or an interruption of the supply of oxygen to the various organs. This anomaly is attenuated by the presence of several lesions (multivessel disease patients), which can lead to several complications. The key of a good medical intervention is the fact of establishing a good diagnosis, in order to decide which lesion requires to be treated. In the diagnosis phase, the clinician uses several techniques, among which angiography is the most popular. Angiography is an X-ray technique to show the inside (the lumen) of blood vessels, in order to identify vessel narrowing: stenosis. Despite its widespread use, angiography is often imperfect in determining the physiological significance of coronary stenosis. If the problem remains simple for non significant lesions ($\leq 40\%$) or very severe ($\geq 70\%$), a very important category of intermediate lesions must benefit from a functional evaluation which will determine the strategy of treatment [80].

The technique of the fractional flow reserve FFR has derived from the initial coronary physical approaches decades ago. Since then, many studies have demonstrated its effectiveness in improving the patients prognosis, by applying the appropriate approach. Its contribution in the reduction of mortality was statistically proved by the FAME (Fractional Flow Reserve Versus Angiography for Multivessel Evaluation) study [158]. It is established that the FFR can be easily measured during coronary angiography by calculating the ratio of distal coronary pressure P_d to aortic pressure P_a. These pressures are measured simultaneously with a special guide-wire. FFR in a normal coronary artery equals to 1.0. FFR value of 0.80 or less identifies ischemia-causing coronary lesions with an accuracy of more than 90% [158].

Obviously, from an interventional point of view, the FFR is binding since it is invasive. It should also be noted that this technique induces additional costs, which are not covered by insurances in several countries. For these reasons, it is used only in less than 10% of the cases.

In this perspective, a new virtual version of the FFR, entitled VFFR, has emerged as an attractive and non-invasive alternative to standard FFR, see [149], [132]. VFFR is based on computational modeling, mainly fluid and fluid-structural dynamics. However, there are key scientific, logistic and commercial challenges that need to be overcome before VFFR can be translated into routine clinical practice.

While most of the studies related to vFFR use Navier-Stokes models, we focus on the non-newtonian case, starting with a generalized fluid flow approach. These models are more relevant for the coronary arteries, and we expect that the computation of the FFR should then be more accurate. We are also leading numerical studies to assess the impact (on the FFR) of the interaction of the physical devices (catheter, optical captors, spheroids) with the blood flow.

4.4. Other application fields

Besides the above mentioned axes, which constitute the project's identity, the methodological tools described in Section have a wider range of application. We currently carry on also the following research actions, in collaboration with external partners.

- **Modeling cell dynamics.** Migration and proliferation of epithelial cell sheets are the two keystone aspects of the collective cell dynamics in most biological processes such as morphogenesis, embryogenesis, cancer and wound healing. It is then of utmost importance to understand their underlying mechanisms.

  Semilinear reaction-diffusion equations are widely used to give a phenomenological description of the temporal and spatial changes occurring within cell populations that undergo scattering (moving), spreading (expanding cell surface) and proliferation. We have followed the same methodology and contributed to assess the validity of such approaches in different settings (cell sheets [111], dorsal closure [49], actin organization [48]). However, epithelial cell-sheet movement is complex enough to undermine most of the mathematical approaches based on *locality*, that is mainly traveling wavefront-like partial differential equations. In [97] it is shown that Madin-Darby Canine Kidney (MDCK) cells extend cryptic lamellipodia to drive the migration, several rows behind the wound edge. In [137] MDCK monolayers are shown to exhibit similar non-local behavior (long range velocity fields, very active border-localized leader cells).

  Our aim is to start from a mesoscopic description of cell interaction: considering cells as independent anonymous agents, we plan to investigate the use of mathematical techniques adapted from the mean-field game theory. Otherwise, looking at them as interacting particles, we will use a multi-agent approach (at least for the actin dynamics). We intend also to consider approaches stemming from compartment-based simulation in the spirit of those developed in [94], [99], [101].

- **Game strategies for thermoelastography.** Thermoelastography is an innovative non-invasive control technology, which has numerous advantages over other techniques, notably in medical imaging [130]. Indeed, it is well known that most pathological changes are associated with changes in tissue stiffness, while remaining isoechoic, and hence difficult to detect by ultrasound techniques. Based on elastic waves and heat flux reconstruction, thermoelastography shows no destructive or aggressive medical sequel, unlike X-ray and comparables techniques, making it a potentially prominent choice for patients.

  Physical principles of thermoelastography originally rely on dynamical structural responses of tissues, but as a first approach, we only consider static responses of linear elastic structures.
  The mathematical formulation of the thermoelasticity reconstruction is based on data completion and material identification, making it a harsh ill posed inverse problem. In previous works [112], [121], we have demonstrated that Nash game approaches are efficient to tackle ill-posedness. We intend to extend the results obtained for Laplace equations in [112], and the algorithms developed in Section 3.1.2.4 to the following problems (of increasing difficulty):
  - Simultaneous data and parameter recovery in linear elasticity, using the so-called Kohn and Vogelius functional (ongoing work, some promising results obtained).

- Data recovery in coupled heat-thermoelasticity systems.
- Data recovery in linear thermoelasticity under stochastic heat flux, where the imposed flux is stochastic.
- Data recovery in coupled heat-thermoelasticity systems under stochastic heat flux, formulated as an incomplete information Nash game.
- Application to robust identification of cracks.

- **Constraint elimination in Quasi-Newton methods.** In single-objective differentiable optimization, Newton's method requires the specification of both gradient and Hessian. As a result, the convergence is quadratic, and Newton's method is often considered as the target reference. However, in applications to distributed systems, the functions to be minimized are usually "functionals", which depend on the optimization variables by the solution of an often complex set of PDE's, through a chain of computational procedures. Hence, the exact calculation of the full Hessian becomes a complex and costly computational endeavor.

  This has fostered the development of *quasi-Newton's methods* that mimic Newton's method but use only the gradient, the Hessian being iteratively constructed by successive approximations inside the algorithm itself. Among such methods, the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm is well-known and commonly employed. In this method, the Hessian is corrected at each new iteration by rank-one matrices defined from several evaluations of the gradient only. The BFGS method has "super-linear convergence".

  For constrained problems, certain authors have developed so-called *Riemannian BFGS*, e.g. [140], that have the desirable convergence property in constrained problems. However, in this approach, the constraints are assumed to be known formally, by explicit expressions.

  In collaboration with ONERA-Meudon, we are exploring the possibility of representing constraints, in successive iterations, through local approximations of the constraint surfaces, splitting the design space locally into tangent and normal sub-spaces, and eliminating the normal coordinates through a linearization, or more generally a finite expansion, and applying the BFGS method through dependencies on the coordinates in the tangent subspace only. Preliminary experiments on the difficult Rosenbrock test-case, although in low dimensions, demonstrate the feasibility of this approach. On-going research is on theorizing this method, and testing cases of higher dimensions.

- **Multi-objective optimization for nanotechnologies.** Our team takes part in a larger collaboration with CEA/LETI (Grenoble), initiated by the Inria Project-Team Nachos, and related to the Maxwell equations. Our component in this activity relates to the optimization of nanophotonic devices, in particular with respect to the control of thermal loads. We have first identified a gradation of representative test-cases of increasing complexity:
  - infrared micro-source;
  - micro-photoacoustic cell;
  - nanophotonic device.

  These cases involve from a few geometric parameters to be optimized to a functional minimization subject to a finite-element solution involving a large number of dof's. CEA disposes of such codes, but considering the computational cost of the objective functions in the complex cases, the first part of our study is focused on the construction and validation of meta-models, typically of RBF-type. Multi-objective optimization will be carried out subsequently by MGDA, and possibly Nash games.

CAGIRE Project-Team

4. Application Domains

4.1. Aeronautics

Cagire is presently involved in studies mainly related to:

- The combustion chamber wall: the modelling, the simulation and the experimentation of the flow around a multiperforated plate representative of a real combustion chamber wall are the three axes we have been developing during the recent period. The continuous improvement of our in-house test facility Maveric is also an important ingredient to produce our own experimental validation data for isothermal flows. For non-isothermal flows, our participation in the EU funded program Soprano will be giving us access to non-isothermal data produced by Onera.
- The flow around airfoils: the modelling of the turbulent boundary layer has been for almost a century a key issue in the aeronautics industry. However, even the more advanced RANS models face difficulties in predicting the influence of pressure gradients on the development of the boundary layer. A main issue is the reliability of the modelling hypotheses, which is crucial for less conservative design. One of the technological barriers is the prediction of the flow in regimes close to the edge of the flight domain (stall, buffeting, unsteady loads) when the boundary layer is slowed down by an adverse pressure gradient. This is the subject of the CIFRE PhD thesis of Gustave Sporschill, started in 2018, in collaboration with Dassault Aviation.

4.2. Power stations

R. Manceau has established a long term collaboration (4 CIFRE PhD theses in the past, 2 ongoing) with the R & D center of EDF of Chatou, for the development of refined turbulence models in the in-house CFD code of EDF, Code_Saturne :

- The prediction of heat transfer in fluid and solid components is of major importance in power stations, in particular, nuclear power plants. Either for the thermohydraulics of the plenum or in the study of accidental scenarii, among others, the accurate estimation of wall heat transfer, mean temperatures and temperature fluctuations are necessary for the evaluation of relevant thermal and mechanical design criteria. The PhD thesis (CIFRE EDF) of G. Mangeon is dedicated to the development of relevant RANS models for these industrial applications.
- Moreover, the prediction of unsteady hydrodynamic loadings is a key point for operating and for safety studies of PWR power plants. Currently, the static loading is correctly predicted by RANS computations but when the flow is transient (as, for instance, in Reactor Coolant Pumps, due to rotor/stator interactions, or during operating transients) or in the presence of large, energetic, coherent structures in the external flow region, the RANS approach is not sufficient, whereas LES is still too costly for a wide use in industry. This issue constitutes the starting point of the just-started PhD thesis (CIFRE EDF) of Vladimir Duffal.

4.3. Automotive propulsion

- The engine (underhood) compartment is a key component of vehicle design, in which the temperature is monitored to ensure the effectiveness and safety of the vehicle, and participates in 5 to 8% of the total drag and CO2 emissions. Dimensioning is an aerodynamic and aerothermal compromise, validated on a succession of road stages at constant speed and stopped phases (red lights, tolls, traffic jam). Although CFD is routinely used for forced convection, state-of-the-art turbulence models are not able to reproduce flows dominated by natural convection during stopped phases, with a Rayleigh number of the order of 10^{10}, such that the design still relies on costly, full-scale, wind tunnel experiments. This technical barrier must be lifted, since the ambition of the PSA group is to reach a *full digital design of their vehicles in the 2025 horizon*, i.e., to almost entirely rely on CFD. This issue is the focus of the ongoing PhD thesis (CIFRE PSA) of S. Jameel, supervised by R. Manceau, and also a part of the ANR project MONACO_2025 described in section 9.2.2 .

- The Power & Vehicles Division of IFPEN co-develops a CFD code to simulate the internal flow in a spark-ignition engine, in order to provide the automotive industry with tools to optimize the design of combustion engines. The RANS method, widely used in the industry, is not sufficiently reliable for quantitative predictions, and is only used as a tool to qualitatively compare different geometries. On the other hand, LES provides more detailed and accurate information, but at the price of a CPU cost unafordable for daily use in the industry. Therefore, IFPEN aims at developing the hybrid RANS/LES methodology, in order to combine the strengths of the two approaches. The PhD thesis of Hassan Afailal, co-supervised by Rémi Manceau, is focused on this issue.

CARDAMOM Project-Team

4. Application Domains

4.1. De-anti icing systems

Impact of large ice debris on downstream aerodynamic surfaces and ingestion by aft mounted engines must be considered during the aircraft certification process. It is typically the result of ice accumulation on unprotected surfaces, ice accretions downstream of ice protected areas, or ice growth on surfaces due to delayed activation of ice protection systems (IPS) or IPS failure. This raises the need for accurate ice trajectory simulation tools to support pre-design, design and certification phases while improving cost efficiency. Present ice trajectory simulation tools have limited capabilities due to the lack of appropriate experimental aerodynamic force and moment data for ice fragments and the large number of variables that can affect the trajectories of ice particles in the aircraft flow field like the shape, size, mass, initial velocity, shedding location, etc... There are generally two types of model used to track shed ice pieces. The first type of model makes the assumption that ice pieces do not significantly affect the flow. The second type of model intends to take into account ice pieces interacting with the flow. We are concerned with the second type of models, involving fully coupled time-accurate aerodynamic and flight mechanics simulations, and thus requiring the use of high efficiency adaptive tools, and possibly tools allowing to easily track moving objects in the flow. We will in particular pursue and enhance our initial work based on adaptive immerse boundary capturing of moving ice debris, whose movements are computed using basic mechanical laws.

In [51] it has been proposed to model ice shedding trajectories by an innovative paradigm that is based on CArtesian grids, PEnalization and LEvel Sets (LESCAPE code). Our objective is to use the potential of high order unstructured mesh adaptation and immersed boundary techniques to provide a geometrically flexible extension of this idea. These activities will be linked to the development of efficient mesh adaptation and time stepping techniques for time dependent flows, and their coupling with the immersed boundary methods we started developing in the FP7 EU project STORM [45], [100]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [73], [89], [90]. From the numerical point of view one of the major challenges is to guarantee efficiency and accuracy of the time stepping in presence of highly stretched adaptive and moving meshes. Semi-implicit, locally implicit, multi-level, and split discretizations will be explored to this end.

Besides the numerical aspects, we will deal with modelling challenges. One source of complexity is the initial conditions which are essential to compute ice shedding trajectories. It is thus extremely important to understand the mechanisms of ice release. With the development of next generations of engines and aircraft, there is a crucial need to better assess and predict icing aspects early in design phases and identify breakthrough technologies for ice protection systems compatible with future architectures. When a thermal ice protection system is activated, it melts a part of the ice in contact with the surface, creating a liquid water film and therefore lowering ability of the ice block to adhere to the surface. The aerodynamic forces are then able to detach the ice block from the surface [53]. In order to assess the performance of such a system, it is essential to understand the mechanisms by which the aerodynamic forces manage to detach the ice. The current state of the art in icing codes is an empirical criterion. However such an empirical criterion is unsatisfactory. Following the early work of [56], [50] we will develop appropriate asymptotic PDE approximations allowing to describe the ice formation and detachment, trying to embed in this description elements from damage/fracture mechanics. These models will constitute closures for aerodynamics/RANS and URANS simulations in the form of PDE wall models, or modified boundary conditions.

In addition to this, several sources of uncertainties are associated to the ice geometry, size, orientation and the shedding location. In very few papers [104], some sensitivity analysis based on Monte Carlo method have been conducted to take into account the uncertainties of the initial conditions and the chaotic nature of the ice particle motion. We aim to propose some systematic approach to handle every source of uncertainty in an efficient way relying on some state-of-art techniques developed in the Team. In particular, we will perform an uncertainty propagation of some uncertainties on the initial conditions (position, orientation, velocity,...) through a low-fidelity model in order to get statistics of a multitude of particle tracks. This study will be done in collaboration with ETS (Ecole de Technologies Supérieure, Canada). The longterm objective is to produce footprint maps and to analyse the sensitivity of the models developed.

4.2. Space re-entry

As already mentioned, atmospheric re-entry involves multi-scale fluid flow physics including highly rarefied effects, aerothermochemistry, radiation. All this must be coupled to the response of thermal protection materials to extreme conditions. This response is most often the actual objective of the study, to allow the certification of Thermal Protection Systems (TPS).

One of the applications we will consider is the so-called post-flight analysis of a space mission. This involves reconstructing the history of the re-entry module (trajectory and flow) from data measured on the spacecraft by means of a Flush Air Data System (FADS), a set of sensors flush mounted in the thermal protection system to measure the static pressure (pressure taps) and heat flux (calorimeters). This study involves the accurate determination of the freestream conditions during the trajectory. In practice this means determining temperature, pressure, and Mach number in front of the bow shock forming during re-entry. As shown by zur Nieden and Olivier [121], state of the art techniques for freestream characterization rely on several approximations, such as e.g. using an equivalent calorically perfect gas formulas instead of taking into account the complex aero-thermo-chemical behaviour of the fluid. These techniques do not integrate measurement errors nor the heat flux contribution, for which a correct knowledge drives more complex models such as gas surface interaction. In this context, CFD supplied with UQ tools permits to take into account chemical effects and to include both measurement errors and epistemic uncertainties, e.g. those due to the fluid approximation, on the chemical model parameters in the bulk and at the wall (surface catalysis).

Rebuilding the freestream conditions from the stagnation point data therefore amounts to solving a stochastic inverse problem, as in robust optimization. Our objective is to build a robust and global framework for rebuilding freestream conditions from stagnation-point measurements for the trajectory of a re-entry vehicle. To achieve this goal, methods should be developed for

- an accurate simulation of the flow in all the regimes, from rarefied, to transitional, to continuous ;
- providing a complete analysis about the reliability and the prediction of the numerical simulation in hypersonic flows, determining the most important source of error in the simulation (PDE model, discretization, mesh, etc)
- reducing the overall computational cost of the analysis .

Our work on the improvement of the simulation capabilities for re-entry flows will focus both on the models and on the methods. We will in particular provide an approach to extend the use of standard CFD models in the transitional regime, with CPU gains of several orders of magnitude w.r.t. Boltzmann solvers. To do this we will use the results of a boundary layer analysis allowing to correct the Navier-Stokes equations. This theory gives modified (or extended) boundary conditions that are called "slip velocity" and "temperature jump" conditions. This theory seems to be completely ignored by the aerospace engineering community. Instead, people rather use a simpler theory due to Maxwell that also gives slip and jump boundary conditions: however, the coefficients given by this theory are not correct. This is why several teams have tried to modify these coefficients by some empirical methods, but it seems that this does not give any satisfactory boundary conditions.

Our project is twofold. First, we want to revisit the asymptotic theory, and to make it known in the aerospace community. Second, we want to make an intensive sensitivity analysis of the model to the various coefficients of the boundary conditions. Indeed, there are two kinds of coefficients in these boundary conditions. The first one is the accomodation coefficient: in the kinetic model, it gives the proportion of molecules that are specularly reflected, while the others are reflected according to a normal distribution (the so-called diffuse reflexion). This coefficient is a data of the kinetic model that can be measured by experiments: it depends on the material and the structure of the solid boundary, and of the gas. Its influence on the results of a Navier-Stokes simulation is certainly quite important. The other coefficients are those of the slip and jump boundary conditions: they are issued from the boundary layer analysis, and we have absolutely no idea of the order of magnitude of their influence on the results of a Navier-Stokes solution. In particular, it is not clear if these results are more sensitive to the accomodation coefficient or to these slip and jump coefficients.

In this project, we shall make use of the expertise of the team on uncertainty quantification to investigate the sensitivity of the Navier-Stokes model with slip and jump coefficients to these various coefficients. This would be rather new in the field of aerospace community. It could also have some impacts in other sciences in which slip and jump boundary conditions with incorrect coefficients are still used, like for instance in spray simulations: for very small particles immersed in a gas, the drag coefficient is modified to account for rarefied effects (when the radius of the particle is of the same order of magnitude as the mean free path in the gas), and slip and jump boundary conditions are used.
Another application which has very close similarities to the physics of de-anti icing systems is the modelling of the solid and liquid ablation of the thermal protective system of the aircraft. This involves the degradation and recession of the solid boundary of the protection layer due to the heating generated by the friction. As in the case of de-anti icing systems, the simulation of these phenomena need to take into account the heat conduction in the solid, its phase change, and the coupling between a weakly compressible and a compressible phase. Fluid/Solid coupling methods are generally based on a weak approach. Here we will both study, by theoretical and numerical techniques, a strong coupling method for the interaction between the fluid and the solid, and, as for de-anti icing systems, attempt at developing appropriate asymptotic models. These would constitute some sort of thin layer/wall models to couple to the external flow solver.

These modelling capabilities will be coupled to high order adaptive discretizations to provide high fidelity flow models. One of the most challenging problems is the minimization of the influence of mesh and scheme on the wall conditions on the re-entry module. To reduce this influence, we will investigate both high order adaptation across the bow shock, and possibly adaptation based on uncertainty quantification high order moments related to the heat flux estimation, or shock fitting techniques [54], [95]. These tools will be coupled to our robust inverse techniques. One of our objectives is to development of a low-cost strategy for improving the numerical prediction by taking into account experimental data. Some methods have been recently introduced [103] for providing an estimation of the numerical errors/uncertainties. We will use some metamodels for solving the inverse problem, by considering all sources of uncertainty, including those on physical models. We will validate the framework sing the experimental data available in strong collaboration with the von Karman Institute for Fluid dynamics (VKI). In particular, data coming from the VKI Longshot facility will be used. We will show application of the developed numerical tool for the prediction in flight conditions.

These activities will benefit from our strong collaborations with the CEA and with the von Karman Institute for Fluid Dynamics and ESA.

4.3. Energy

We will develop modelling and design tools, as well as dedicated platforms, for Rankine cycles using complex fluids (organic compounds), and for wave energy extraction systems.

Organic Rankine Cycles (ORCs) use heavy organic compounds as working fluids. This results in superior efficiency over steam Rankine cycles for source temperatures below 900 K. ORCs typically require only a single-stage rotating component making them much simpler than typical multi-stage steam turbines. The strong pressure reduction in the turbine may lead to supersonic flows in the rotor, and thus to the appearance of shocks, which reduces the efficiency due to the associated losses. To avoid this, either a larger multi stage installation is used, in which smaller pressure drops are obtained in each stage, or centripetal turbines are used, at very high rotation speeds (of the order of 25,000 rpm). The second solution allows to keep the simplicity of the expander, but leads to poor turbine efficiencies (60-80%) - w.r.t. modern, highly optimized, steam and gas turbines - and to higher mechanical constraints. The use of *dense-gas working fluids*, *i.e.* operating close to the saturation curve, in properly chosen conditions could increase the turbine critical Mach number avoiding the formation of shocks, and increasing the efficiency. Specific shape optimization may enhance these effects, possibly allowing the reduction of rotation speeds. However, dense gases may have significantly different properties with respect to dilute ones. Their dynamics is governed by a thermodynamic parameter known as the fundamental derivative of gas dynamics

$$\Gamma = 1 + \frac{\rho}{c}\left(\frac{\partial c}{\partial \rho}\right)_s, \tag{1}$$

where ρ is the density, c is the speed of sound and s is the entropy. For ideal gas $\Gamma = (\gamma + 1)/2 > 1$. For some complex fluids and some particular conditions of pressure and temperature, Γ may be lower that one, implying that $(\partial c/\partial \rho)_s < 0$. This means that the acceleration of pressure perturbations through a variable density fluids may be reversed and become a deceleration. It has been shown that, for $\Gamma << 1$, compression shocks are strongly reduced, thus alleviating the shock intensity. This has great potential in increasing the efficiency. This is why so much interest is put on dense gas ORCs.

The simulation of these gases requires accurate thermodynamic models, such as Span-Wagner or Peng-Robinson (see [66]). The data to build these models is scarce due to the difficulty of performing reliable experiments. The related uncertainty is thus very high. Our work will go in the following directions:

1. develop deterministic models for the turbine and the other elements of the cycle. These will involve multi-dimensional high fidelity, as well as intermediate and low fidelity (one- and zero-dimensional), models for the turbine, and some 0D/1D models for other element of the cycle (pump, condenser, etc) ;
2. validation of the coupling between the various elements. The following aspects will be considered: characterization of the uncertainties on the cycle components (e.g. empirical coefficients modelling the pump or the condenser), calibration of the thermodynamic parameters, model the uncertainty of each element, and the influence of the unsteady experimental data ;
3. demonstrate the interest of a specific optimization of geometry, operating conditions, and the choice of the fluid, according to the geographical location by including local solar radiation data. Multi-objective optimization will be considered to maximize performance indexes (e.g. Carnot efficiency, mechanical work and energy production), and to reduce the variability of the output.

This work will provide modern tools for the robust design of ORCs systems. It benefits from the direct collaboration with the SME EXOES (ANR LAbCom VIPER), and from a collaboration with LEMMA.

Wave energy conversion is an emerging sector in energy engineering. The design of new and efficient Wave Energy Converters (WECs) is thus a crucial activity. As pointed out by Weber [120], it is more economical to raise the technology performance level (TPL) of a wave energy converter concept at low technology readiness level (TRL). Such a development path puts a greater demand on the numerical methods used. The findings of Weber also tell us that important design decisions as well as optimization should be performed as early in the development process as possible. However, as already mentioned, today the wave energy sector relies heavily on the use of tools based on simplified linear hydrodynamic models for the prediction of motions, loads, and power production. Our objective is to provide this sector, and especially SMEs, with robust design tools to minimize the uncertainties in predicted power production, loads, and costs of wave energy.

Following our initial work [76], we will develop, analyse, compare, and use for multi-fidelity optimization,non-linear models of different scales (fidelity) ranging from simple linear hydrodynamics over asymptotic discrete nonlinear wave models, to non-hydrostatic anisoptropic Euler free surface solvers. We will not work on the development of small scale models (VOF-RANS or LES) but may use such models, developed by our collaborators, for validation purposes. These developments will benefit from all our methodological work on asymptotic modelling and high order discretizations. As shown in [76], asymptotic models foe WECs involve an equation for the pressure on the body inducing a PDE structure similar to that of incompressible flow equations. The study of appropriate stable and efficient high order approximations (coupling velocity-pressure, efficient time stepping) will be an important part of this activity. Moreover, the flow-floating body interaction formulation introduces time stepping issues similar to those encountered in fluid structure interaction problems, and require a clever handling of complex floater geometries based on adaptive and ALE techniques. For this application, the derivation of fully discrete asymptotics may actually simplify our task.

Once available, we will use this hierarchy of models to investigate and identify the modelling errors, and provide a more certain estimate of the cost of wave energy. Subsequently we will look into optimization cycles by comparing time-to-decision in a multi-fidelity optimization context. In particular, this task will include the development and implementation of appropriate surrogate models to reduce the computational cost of expensive high fidelity models. Here especially artificial neural networks (ANN) and Kriging response surfaces (KRS) will be investigated. This activity on asymptotic non-linear modelling for WECs, which has had very little attention in the past, will provide entirely new tools for this application. Multi-fidelity robust optimization is also an approach which has never been applied to WECs.

This work is the core of the EU OCEANEranet MIDWEST project, which we coordinate. It will be performed in collaboration with our European partners, and with a close supervision of European SMEs in the sector, which are part of the steering board of MIDWEST (WaveDragon, Waves4Power, Tecnalia).

4.4. Materials engineering

Because of their high strength and low weight, ceramic-matrix composite materials (CMCs) are the focus of active research for aerospace and energy applications involving high temperatures, either military or civil. Though based on brittle ceramic components, these composites are not brittle due to the use of a fibre/matrix interphase that preserves the fibres from cracks appearing in the matrix. Recent developments aim at implementing also in civil aero engines a specific class of Ceramic Matrix Composite materials (CMCs) that show a self-healing behaviour. Self-healing consists in filling cracks appearing in the material with a dense fluid formed in-situ by oxidation of part of the matrix components. Self-healing (SH) CMCs are composed of a complex three-dimensional topology of woven fabrics containing fibre bundles immersed in a matrix coating of different phases. The oxide seal protects the fibres which are sensitive to oxidation, thus delaying failure. The obtained lifetimes reach hundreds of thousands of hours [108].

The behaviour of a fibre bundle is actually extremely variable, as the oxidation reactions generating the self-healing mechanism have kinetics strongly dependent on temperature and composition. In particular, the lifetime of SH-CMCs depends on: (i) temperature and composition of the surrounding atmosphere; (ii) composition and topology of the matrix layers; (iii) the competition of the multidimensional diffusion/oxidation/volatilization processes; (iv) the multidimensional flow of the oxide in the crack; (v) the inner topology of fibre bundles; (vi) the distribution of critical defects in the fibres. Unfortunately, experimental investigations on the full materials are too long (they can last years) and their output too qualitative (the coupled effects can only be observed a-posteriori on a broken sample). Modelling is thus essential to study and to design SH-CMCs.

In collaboration wit the LCTS laboratory (a joint CNRS-CEA-SAFRAN-Bordeaux University lab devoted to the study of thermo-structural materials in Bordeaux), we are developing a multi-scale model in which a structural mechanics solver is coupled with a closure model for the crack physico chemistry. This model is obtained as a multi-dimensional asymptotic crack averaged approximation fo the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [69], [74], [105]. We have demonstrated the potential of this model in showing the importance of taking into account the multi-dimensional topology of a fibre bundle (distribution of fibres) in the rupture mechanism. This means that the 0-dimensional model used in most of the studies (se e.g. [64]) will underestimate appreciably the lifetime of the material. Based on these recent advances, we will further pursue the development of multi-scale multi-dimensional asymptotic closure models for the parametric design of self healing CMCs. Our objectives are to provide: (i) new, non-linear multi-dimensional mathematical model of CMCs, in which the physico-chemistry of the self-healing process is more strongly coupled to the two-phase (liquid gas) hydro-dynamics of the healing oxide ; (ii) a model to represent and couple crack networks ; (iii) a robust and efficient coupling with the structural mechanics code ; (iv) validate this platform with experimental data obtained at the LCTS laboratory. The final objective is to set up a multi-scale platform for the robust prediction of lifetime of SH-CMCs, which will be a helpful tool for the tailoring of the next generation of these materials.

4.5. Coastal and civil engineering

Our objective is to bridge the gap between the development of high order adaptive methods, which has mainly been performed in the industrial context and environmental applications, with particular attention to coastal and hydraulic engineering. We want to provide tools for adaptive non-linear modelling at large and intermediate scales (near shore, estuarine and river hydrodynamics). We will develop multi-scale adaptive models for free surface hydrodynamics. Beside the models and codes themselves, based on the most advanced numerics we will develop during this project, we want to provide sufficient know how to control, adapt and optimize these tools.

We will focus our effort in the understanding of the interactions between asymptotic approximations and numerical approximations. This is extremely important in at least two aspects. The first is the capability of a numerical model to handle highly dispersive wave propagation. This is usually done by high accuracy asymptotic PDE expansions. Here we plan to make heavily use of our results concerning the relations between vertical asymptotic expansions and standard finite element approximations. In particular, we will invest some effort in the development of xy+z adaptive finite element approximations of the incompressible Euler equations. Local $p-$adaptation of the vertical approximation may provide a “variable depth” approximation exploiting numerics instead of analytical asymptotics to control the physical behaviour of the model.

Another important aspect which is not understood well enough at the moment is the role of dissipation in wave breaking regions. There are several examples of breaking closure, going from algebraic and PDE-based eddy viscosity methods [86], [110], [102], [71], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [114], [115], [113], [84], [77]. In both cases, numerical dissipation plays an important role and the activation or not of the breaking closure, as the quantitative contribution of numerical dissipation to the flow has not been properly investigated. These elements must be clarified to allow full control of adaptive techniques for the models used in this type of applications.

Another point we want to clarify is how to optimize the discretization of asymptotic PDE models. In particular, when adding mesh size(s) and time step, we are in presence of at least 3 (or even more) small parameters. The relations between physical ones have been more or less investigates, as have been the ones between purely numerical ones. We plan to study the impact of numerics on asymptotic PDE modelling by reverting the usual process and studying asymptotic limits of finite element discretizations of the Euler equations. Preliminary results show that this does allow to provide some understanding of this interaction and to possibly propose considerably improved numerical methods [52].

DEFI Project-Team

4. Application Domains

4.1. Radar and GPR applications

Conventional radar imaging techniques (ISAR, GPR, etc.) use backscattering data to image targets. The commonly used inversion algorithms are mainly based on the use of weak scattering approximations such as the Born or Kirchhoff approximation leading to very simple linear models, but at the expense of ignoring multiple scattering and polarization effects. The success of such an approach is evident in the wide use of synthetic aperture radar techniques.

However, the use of backscattering data makes 3-D imaging a very challenging problem (it is not even well understood theoretically) and as pointed out by Brett Borden in the context of airborne radar: “In recent years it has become quite apparent that the problems associated with radar target identification efforts will not vanish with the development of more sensitive radar receivers or increased signal-to-noise levels. In addition it has (slowly) been realized that greater amounts of data - or even additional “kinds” of radar data, such as added polarization or greatly extended bandwidth - will all suffer from the same basic limitations affiliated with incorrect model assumptions. Moreover, in the face of these problems it is important to ask how (and if) the complications associated with radar based automatic target recognition can be surmounted.” This comment also applies to the more complex GPR problem.

Our research themes will incorporate the development, analysis and testing of several novel methods, such as sampling methods, level set methods or topological gradient methods, for ground penetrating radar application (imaging of urban infrastructures, landmines detection, underground waste deposits monitoring,) using multistatic data.

4.2. Biomedical imaging

Among emerging medical imaging techniques we are particularly interested in those using low to moderate frequency regimes. These include Microwave Tomography, Electrical Impedance Tomography and also the closely related Optical Tomography technique. They all have the advantage of being potentially safe and relatively cheap modalities and can also be used in complementarity with well established techniques such as X-ray computed tomography or Magnetic Resonance Imaging.

With these modalities tissues are differentiated and, consequentially can be imaged, based on differences in dielectric properties (some recent studies have proved that dielectric properties of biological tissues can be a strong indicator of the tissues functional and pathological conditions, for instance, tissue blood content, ischemia, infarction, hypoxia, malignancies, edema and others). The main challenge for these functionalities is to built a 3-D imaging algorithm capable of treating multi-static measurements to provide real-time images with highest (reasonably) expected resolutions and in a sufficiently robust way.

Another important biomedical application is brain imaging. We are for instance interested in the use of EEG and MEG techniques as complementary tools to MRI. They are applied for instance to localize epileptic centers or active zones (functional imaging). Here the problem is different and consists into performing passive imaging: the epileptic centers act as electrical sources and imaging is performed from measurements of induced currents. Incorporating the structure of the skull is primordial in improving the resolution of the imaging procedure. Doing this in a reasonably quick manner is still an active research area, and the use of asymptotic models would offer a promising solution to fix this issue.

4.3. Non destructive testing and parameter identification

One challenging problem in this vast area is the identification and imaging of defaults in anisotropic media. For instance this problem is of great importance in aeronautic constructions due to the growing use of composite materials. It also arises in applications linked with the evaluation of wood quality, like locating knots in timber in order to optimize timber-cutting in sawmills, or evaluating wood integrity before cutting trees. The anisotropy of the propagative media renders the analysis of diffracted waves more complex since one cannot only relies on the use of backscattered waves. Another difficulty comes from the fact that the micro-structure of the media is generally not well known a priori.

Our concern will be focused on the determination of qualitative information on the size of defaults and their physical properties rather than a complete imaging which for anisotropic media is in general impossible. For instance, in the case of homogeneous background, one can link the size of the inclusion and the index of refraction to the first eigenvalue of so-called interior transmission problem. These eigenvalues can be determined form the measured data and a rough localization of the default. Our goal is to extend this kind of idea to the cases where both the propagative media and the inclusion are anisotropic. The generalization to the case of cracks or screens has also to be investigated.

In the context of nuclear waste management many studies are conducted on the possibility of storing waste in a deep geological clay layer. To assess the reliability of such a storage without leakage it is necessary to have a precise knowledge of the porous media parameters (porosity, tortuosity, permeability, etc.). The large range of space and time scales involved in this process requires a high degree of precision as well as tight bounds on the uncertainties. Many physical experiments are conducted in situ which are designed for providing data for parameters identification. For example, the determination of the damaged zone (caused by excavation) around the repository area is of paramount importance since microcracks yield drastic changes in the permeability. Level set methods are a tool of choice for characterizing this damaged zone.

4.4. Diffusion MRI

In biological tissues, water is abundant and magnetic resonance imaging (MRI) exploits the magnetic property of the nucleus of the water proton. The imaging contrast (the variations in the grayscale in an image) in standard MRI can be from either proton density, T1 (spin-lattice) relaxation, or T2 (spin-spin) relaxation and the contrast in the image gives some information on the physiological properties of the biological tissue at different physical locations of the sample. The resolution of MRI is on the order of millimeters: the greyscale value shown in the imaging pixel represents the volume-averaged value taken over all the physical locations contained that pixel.

In diffusion MRI, the image contrast comes from a measure of the average distance the water molecules have moved (diffused) during a certain amount of time. The Pulsed Gradient Spin Echo (PGSE) sequence is a commonly used sequence of applied magnetic fields to encode the diffusion of water protons. The term 'pulsed' means that the magnetic fields are short in duration, an the term gradient means that the magnetic fields vary linearly in space along a particular direction. First, the water protons in tissue are labelled with nuclear spin at a precession frequency that varies as a function of the physical positions of the water molecules via the application of a pulsed (short in duration, lasting on the order of ten milliseconds) magnetic field. Because the precessing frequencies of the water molecules vary, the signal, which measures the aggregate phase of the water molecules, will be reduced due to phase cancellations. Some time (usually tens of milliseconds) after the first pulsed magnetic field, another pulsed magnetic field is applied to reverse the spins of the water molecules. The time between the applications of two pulsed magnetic fields is called the 'diffusion time'. If the water molecules have not moved during the diffusion time, the phase dispersion will be reversed, hence the signal loss will also be reversed, the signal is called refocused. However, if the molecules have moved during the diffusion time, the refocusing will be incomplete and the signal detected by the MRI scanner if weaker than if the water molecules have not moved. This lack of complete refocusing is called the signal attenuation and is the basis of the image contrast in DMRI. the pixels showning more signal attenuation is associated with further water displacement during the diffusion time, which may be linked to physiological factors, such as higher cell membrane permeability, larger cell sizes, higher extra-cellular volume fraction.

We model the nuclear magnetization of water protons in a sample due to diffusion-encoding magnetic fields by a multiple compartment Bloch-Torrey partial differential equation, which is a diffusive-type time-dependent PDE. The DMRI signal is the integral of the solution of the Bloch-Torrey PDE. In a homogeneous medium, the intrinsic diffusion coeffcient D will appear as the slope of the semi-log plot of the signal (in approporiate units). However, because during typical scanning times, 50-100ms, water molecules have had time to travel a diffusion distance which is long compared to the average size of the cells, the slope of the semi-log plot of the signal is in fact a measure of an 'effective' diffusion coefficient. In DMRI applications, this measured quantity is called the 'apparent diffusion coefficient' (ADC) and provides the most commonly used form the image contrast for DMRI. This ADC is closely related to the effective diffusion coefficient obtainable from mathematical homogenization theory.

4.5. Fluid flow applications

Specific actions are devoted to the problem of atmospheric reentry simulations. We focus on several aspects : i) on the development of innovative algorithms improving the prediction of hypersonic flows and including system uncertainties, ii) on the application of these methods to the atmospheric reentry of space vehicles for the control and the optimization of the trajectory, iii) on the debris reentry, which is of fundamental importance for NASA, CNES and ESA. Several works are already initiated with funding from CNES, Thales, and ASL. An ongoing activity concerns the design of the Thermal Protection System (TPS) that shields the spacecraft from aerothermal heating, generated by friction at the surface of the vehicle. The TPS is usually composed of different classes of materials, depending on the mission and the planned trajectory. One major issue is to model accurately the material response to ensure a safe design. High-fidelity material modeling for ablative materials has been developed by NASA, but a lot of work is still needed concerning the assessment of physical and modeling uncertainties during the design process. Our objective is to set up a predictive numerical tool to reliably estimate the response of ablative materials for different aerothermal conditions.

An important effort is dedicated to the simulation of fluids featuring complex thermodynamic behavior, in the context of two distinct projects: the VIPER project, funded by Aquitaine Region, and a project with CWI (Scientific Computing Group). Dense gases (DGs) are defined as single-phase vapors operating at temperatures and pressures conditions close to the saturation curve. The interest in studying complex dynamics of compressible dense gas flows comes from the potential technological advantages of using these fluids in energy conversion cycles, such as in Organic Rankine Cycles (ORCs) which used dense gases as energy converters for biomass fuels and low-grade heat from geothermal or industrial waste heat sources. Since these fluids feature large uncertainties in their estimated thermodynamic properties (critical properties, acentric factor, etc.), a meaningful numerical prediction of the performance must necessarily take into account these uncertainties. Other sources of uncertainties include, but are not limited to, the inlet boundary conditions which are often unknown in dense gases applications. Moreover, a robust optimization must also include the more generic uncertainty introduced by the machining tolerance in the construction of the turbine blades.

ECUADOR Project-Team

4. Application Domains

4.1. Algorithmic Differentiation

Algorithmic Differentiation of programs gives sensitivities or gradients, useful for instance for :

- optimum shape design under constraints, multidisciplinary optimization, and more generally any algorithm based on local linearization,
- inverse problems, such as parameter estimation and in particular 4Dvar data assimilation in climate sciences (meteorology, oceanography),
- first-order linearization of complex systems, or higher-order simulations, yielding reduced models for simulation of complex systems around a given state,
- adaption of parameters for classification tools such as Machine Learning systems, in which Adjoint Differentiation is also known as *backpropagation*.
- mesh adaptation and mesh optimization with gradients or adjoints,
- equation solving with the Newton method,
- sensitivity analysis, propagation of truncation errors.

4.2. Multidisciplinary optimization

A CFD program computes the flow around a shape, starting from a number of inputs that define the shape and other parameters. On this flow one can define optimization criteria e.g. the lift of an aircraft. To optimize a criterion by a gradient descent, one needs the gradient of the criterion with respect to all inputs, and possibly additional gradients when there are constraints. Adjoint AD is the most efficient way to compute these gradients.

4.3. Inverse problems and Data Assimilation

Inverse problems aim at estimating the value of hidden parameters from other measurable values, that depend on the hidden parameters through a system of equations. For example, the hidden parameter might be the shape of the ocean floor, and the measurable values of the altitude and velocities of the surface. Figure 1 shows an example of an inverse problem using the glaciology code ALIF (a pure C version of ISSM [27]) and its AD-adjoint produced by Tapenade.

One particular case of inverse problems is *data assimilation* [28] in weather forecasting or in oceanography. The quality of the initial state of the simulation conditions the quality of the prediction. But this initial state is not well known. Only some measurements at arbitrary places and times are available. A good initial state is found by solving a least squares problem between the measurements and a guessed initial state which itself must verify the equations of meteorology. This boils down to solving an adjoint problem, which can be done though AD [30]. The special case of *4Dvar* data assimilation is particularly challenging. The 4^{th} dimension in "4D" is time, as available measurements are distributed over a given assimilation period. Therefore the least squares mechanism must be applied to a simulation over time that follows the time evolution model. This process gives a much better estimation of the initial state, because both position and time of measurements are taken into account. On the other hand, the adjoint problem involved is more complex, because it must run (backwards) over many time steps. This demanding application of AD justifies our efforts in reducing the runtime and memory costs of AD adjoint codes.

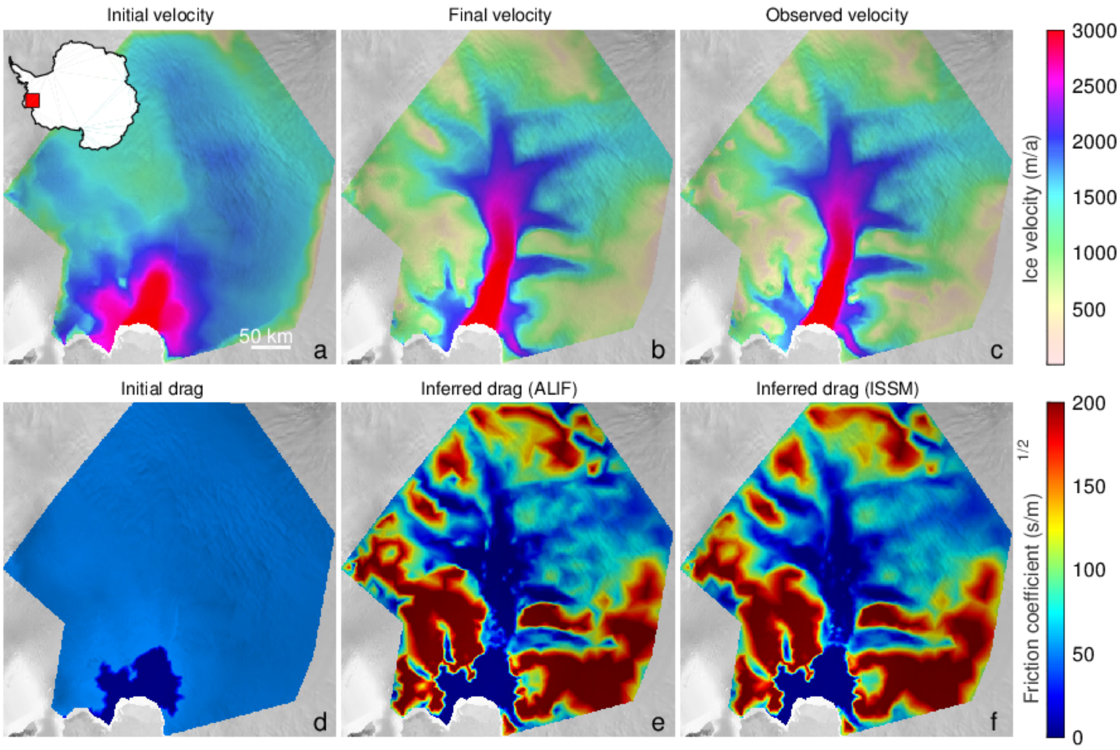


Figure 1. Assimilation of the basal friction under Pine Island glacier, West Antarctica. The final simulated surface velocity (b) is made to match the observed surface velocity (c), by estimation of the basal friction (e). A reference basal friction (f) is obtained by another data assimilation using the hand=written adjoint of ISSM

4.4. Linearization

Simulating a complex system often requires solving a system of Partial Differential Equations. This can be too expensive, in particular for real-time simulations. When one wants to simulate the reaction of this complex system to small perturbations around a fixed set of parameters, there is an efficient approximation: just suppose that the system is linear in a small neighborhood of the current set of parameters. The reaction of the system is thus approximated by a simple product of the variation of the parameters with the Jacobian matrix of the system. This Jacobian matrix can be obtained by AD. This is especially cheap when the Jacobian matrix is sparse. The simulation can be improved further by introducing higher-order derivatives, such as Taylor expansions, which can also be computed through AD. The result is often called a *reduced model*.

4.5. Mesh adaptation

Some approximation errors can be expressed by an adjoint state. Mesh adaptation can benefit from this. The classical optimization step can give an optimization direction not only for the control parameters, but also for the approximation parameters, and in particular the mesh geometry. The ultimate goal is to obtain optimal control parameters up to a precision prescribed in advance.

ELAN Team

4. Application Domains

4.1. Mechanical Engineering

Many physicists and mathematicians have strived for centuries to understand the principles governing those complex mechanical phenomena, providing a number of continuous models for slender structures, granular matter, and frictional contact. In the XX$^{\text{th}}$ century, industrial applications such as process automatization and new ways of transportation have boosted the fields of Mechanical Engineering and Computer-Aided Design, where material strength, reliability of mechanisms, and safety, standed for the main priorities. Instead, large displacements of structures, buckling, tearing, or entanglement, and even dynamics, were long considered as undesirable behaviors, thus restraining the search for corresponding numerical models.

Only recently, the engineering industry has shown some new and growing interest into the modeling of dynamic phenomena prone to large displacements, contact and friction. For instance, the cosmetology industry is more and more interested in understanding the nonlinear deformation of hair and skin, with the help of simulation. Likewise, auto and aircraft manufacturers are facing new challenges involving buckling or entanglement of thin structures such as carbon or optical fibers; they clearly lack predictive, robust and efficient numerical tools for simulating and optimizing their new manufacturing process, which share many common features with the large-scale simulation scenarii traditionally studied in Computer Graphics applications.

4.2. Computer Graphics

In contrast, Computer Graphics, which has emerged in the 60's with the advent of modern computers, was from the very beginning eager to capture such peculiar phenomena, with the sole aim to produce spectacular images and create astonishing stories. At the origin, Computer Graphics thus drastically departed from other scientific fields. Everyday-life phenomena such as cloth buckling, paper tearing, or hair fluttering in the wind, mostly ignored by other scientists at that time, became actual topics of interest, involving a large set of new research directions to be explored, both in terms of modelling and simulation. Nowadays, although the image production still remains the core activity of the Computer Graphics community, more and more research studies are directed through the virtual and real prototyping of mechanical systems, notably driven by a myriad of new applications in the virtual try on industry (e.g., hairstyling and garment fitting). Furthermore, the advent of additive fabrication is currently boosting research in the free design of new mechanisms or systems for various applications, from architecture design and fabrication of metamaterials to the creation of new locomotion modes in robotics. Some obvious common interests and approaches are thus emerging between Computer Graphics and Mechanical Engineering, yet the two communities remain desperately compartmentalized.

4.3. Soft Matter Physics

From the physics-based viewpoint, since a few decades a new generation of physicists became interested again in the understanding of such visually fascinating phenomena, and started investigating the tight links between geometry and elasticity [0]. Common objects such as folded or torn paper, twined plants, coiled honey threads, or human hair have thus regained some popularity among the community in Nonlinear Physics [0]. In consequence, phenomena of interest have become remarkably close to those of Computer Graphics, since scientists in both places share the common goal to model complex and integrated mechanical phenomena at the macroscopic

[0] In France this new trend was particularly stimulated by the work of Yves Pomeau, who convinced many young scientists to study the nonlinear physics of common objects such as paper, plants, or hair [24].

[0] It is however amusing to observe that research in these areas is quite successful in obtaining the IG Nobel prize [5], [27], thus still being considered as an exotic research topic by physicists.

scale. Of course, the goals and employed methodologies differ substantially from one community to the other, but showcase some evident complementarity: while computer scientists are eager to learn and understand new physical models, physicists get more and more interested in the numerical tools, in which they perceive not only a means to confirm predictions afterwards, but also a support for testing new hypothesis and exploring scenarios that would be too cumbersome or even impossible to investigate experimentally. Besides, numerical exploration starts becoming a valuable tool for getting insights into the search for analytic solutions, thus fully participating to the modeling stage and physical understanding. However, physicists may be limited to a blind usage of numerical black boxes, which may furthermore not be dedicated to their specific needs. According to us, promoting a science of modeling in numerical physics would thus be a promising and rich avenue for the two research fields. Unfortunately, very scarce cooperation currently exists between the two communities, and large networks of collaboration still need to be set up.

GAMMA3 Project-Team (section vide)

MATHERIALS Project-Team (section vide)

MEMPHIS Project-Team

4. Application Domains

4.1. Energy conversion

We apply the methods developed in our team to the domain of wind engineering and sea-wave converters. In Figure 1 , we show results of a numerical model for a sea-wave energy converter. We here rely on a monolithic model to describe the interaction between the rigid floater, air and water; material properties such as densities, viscosities and rigidity vary across the domain. The appropriate boundary conditions are imposed at interfaces that arbitrarily cross the grid using adapted schemes built thanks to geometrical information computed via level set functions [43]. The background method for fluid-structure interface is the volume penalization method [25] where the level set functions is used to improve the degree of accuracy of the method [3] and also to follow the object. The underlined mathematical model is unsteady, and three dimensional; numerical simulations based on a grid with $\mathcal{O}(10^8)$ degrees of freedom are executed in parallel using 512 CPUs .

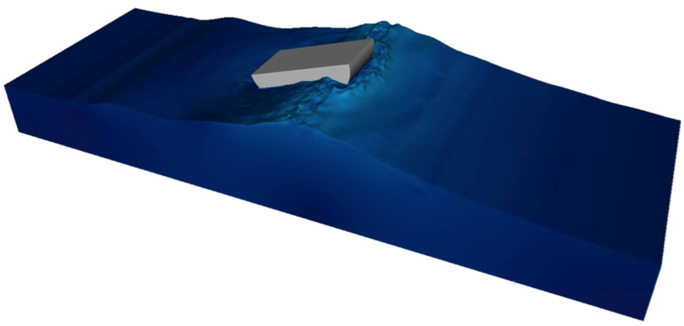


Figure 1. numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.

In the context of the Aerogust (Aeroelastic gust modelling) European project, together with Valorem, we investigated the behavior of wind turbine blades under gust loading. The aim of the project was to optimize the design of wind turbine blades to maximize the power extracted. A meteorological mast (Figure 2 (a)) has been installed in March 2017 in Brittany to measure wind on-site: data provided by the mast have been exploited to initialize the mathematical model. Due to the large cost of the full-order mathematical model, we relied on a simplified model [35] to optimize the global twist. Then, we validated the optimal configuration using the full-order Cartesian model based on the NaSCar solver. Figure 2 (b) shows the flow around the optimized optimized wind turbine rotor.

4.2. Impacts

Mathematical and numerical modelling of physical systems undergoing impacts is challenging due to the presence of large deformations and displacements of the solid part, and due to the strongly non-linear behaviour of the fluid part. At the same time, proper experiments of impact phenomena are particularly dangerous and require expensive facilities, which make them largely impractical. For this reason, there is a growing interest in the development of predictive models for impact phenomena.

Figure 2. Aerogust project. Left: met mast after its installation. Right: flow around the optimized wind turbine rotor (as predicted by NaSCar).

In MEMPHIS, we rely on a fully Eulerian approach based on conservation laws, where the different materials are characterized by their specific constitutive laws, to address these tasks. This approach was introduced in [34] and subsequently pursued and extended in [40], [33], [27], [30] In Figure 3 , we show the results of the numerical simulation of the impact of a copper projectile immersed in air over a copper shield. Results are obtained using a fully parallel monolithic Cartesian method, based on a 4000^2 fixed Cartesian grid. Simulations are performed on a cluster of 512 processors, and benefits from the isomorphism between grid partitioning and processor topology.

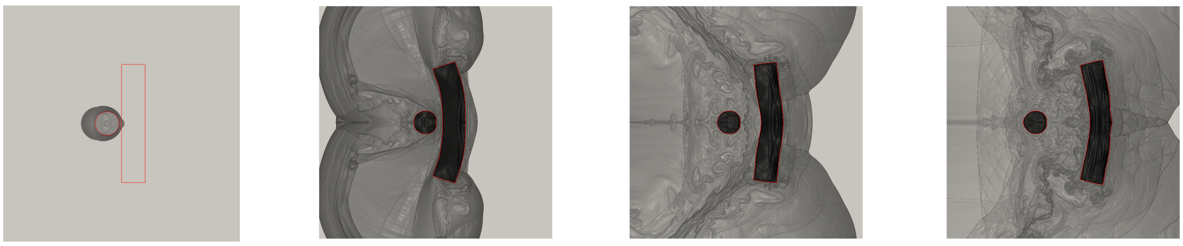


Figure 3. impact and rebound of a copper projectile on a copper plate. Interface and schlieren at $50\mu s$, $199\mu s$, $398\mu s$ and $710\mu s$.

4.3. Vascular flows

A new research direction pursued by the team is the mathematical modelling of vascular blood flows in arteries. Together with the start-up Nurea (http://nurea-soft.com/) and the surgeon Eric Ducasse, we aim at developing reliable and automatic procedures for aneurysm segmentation and for the prediction of aneurysm rupture risk. Our approach exploits two sources of information: (i) numerical simulations of blood flows in complex geometries, based on an octree discretization, and (ii) computed tomography angiography (CTA) data. Figure

4 shows the force distribution on the walls of the abdominal aorta in presence of an aneurysm; results are obtained using a parallelized hierarchical Cartesian scheme based on octrees.

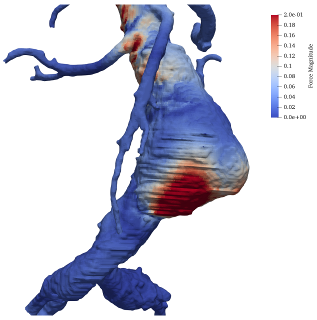


Figure 4. force distribution on the walls of the abdominal aorta in presence of an aneurysm.

MEPHYSTO-POST Team (section vide)

MINGUS Project-Team

4. Application Domains

4.1. Applications

The MINGUS project aims at applying the new numerical methods on realistic problems arising for instance in physics of nanotechnology and physics of plasmas. Therefore, in addition to efforts devoted to the design and the analysis of numerical methods, the inherent large size of the problems at hand requires advanced mathematical and computational methods which are hard to implement. Another application is concerned with population dynamics for which the main goal is to understand how the spatial propagation phenomena affect the demography of a population (plankton, parasite fungi, ...).

Our activity is mostly at an early stage in the process of transfer to industry. However, all the models we use are physically relevant and all have applications in many areas (ITER, Bose-Einstein condensate, wave turbulence, optical tomography, transport phenomena, population dynamics, $\cdots$). As a consequence, our research aims at reaching theoretical physicists or computational scientists in various fields who have strong links with industrial applications.

In order to tackle as realistic physical problems as possible, a fundamental aspect will consist in working on the realization of numerical methods and algorithms which are able to make an efficient use of a large number of processors. Then, it is essential for the numerical methods developed in the MINGuS project to be thought through this prism. We will benefit from the strong expertise of P. Navaro in scientific computing and more precisely on the Selalib software library (see description below).

Below, we detail our main applications: first, the modeling and numerical approximation of magnetized plasmas is our major application and will require important efforts in terms of software developments to scale-up our multiscale methods; second, the transport of charged particles in nanostructures has very interesting applications (like graphene material), for which our contributions will mainly focus on dedicated problems; lastly, applications on population dynamics will be dedicated to mathematical modeling and some numerical validations.

4.1.1. Kinetic problems

The Selalib (SEmi-LAgrangian LIBrary) software library [0] is a modular library for kinetic and gyrokinetic simulations of plasmas in fusion energy devices. Selalib is a collection of fortran modules aimed at facilitating the development of kinetic simulations, particularly in the study of turbulence in fusion plasmas. Selalib offers basic capabilities and modules to help parallelization (both MPI and OpenMP), as well as pre-packaged simulations.

Its main objective is to develop a documented library implementing several numerical methods for the numerical approximation of kinetic models of the form (2). Another objective of the library is to provide physicists with easy-to-use gyrokinetic solvers. It has been originally developed by E. Sonnendrücker and his collaborators in the past CALVI Inria project, and has played an important role in the activities of the IPL FRATRES. P. Navaro is one of the main software engineer of this library and as such he played an important daily role in its development and its portability on supercomputers. Though Selalib has reached a certain maturity some additional works are needed to make available by the community. There are currently discussions for a possible evolution of Selalib, namely the writing of a new release which will be available for free download. Obviously, the team will be involved in this process.

[0] SELALIB, http://selalib.gforge.inria.fr.

At the scientific level, Selalib is of great interest for us since it provides a powerful tool with which we can test, validate and compare our new methods and algorithms (*users level*). Besides numerical algorithms the library provides low-level utilities, input-output modules as well as parallelization strategies dedicated to kinetic problems. Moreover, a collection of simulations for typical test cases (of increasing difficulties) with various discretization schemes supplements the library. This library turns out to be the ideal complement of our activities and it will help us to scale-up our numerical methods to high-dimensional kinetic problems. During the last years, several experiments have been successfully performed in this direction (especially with PhD students) and it is important for us that this approach remains throughout.
Then, we intend to integrate several of the numerical methods developed by the team within the Selalib library, with the strong help of P. Navaro (*contributors level*). This work has important advantages: (i) it will improve our research codes (in terms of efficiency but also of software maintenance point of view); (ii) it will help us to promote our research by making our methods available to the research community.

4.1.2. Quantum problems

Nowadays, a great challenge consists in the downscaling at the nanometer scale of electronic components in order to improve speed and efficiency of semiconductor materials. In this task, modeling and numerical simulations play an important role in the determination of the limit size of the nanotransistors At the nanoscale, quantum effects have to be considered and the Schrödinger equation (1) is prominent equation in this context. In the so-called semiclassical regime or when the transport is strongly confined, the solution endows space-time highly oscillations which are very difficult to capture numerically.

An important application is the modeling of charged particles transport in graphene. Graphene is a sheet of carbone made of a single layer of molecule, organised in a bidimensional honeycomb crystal. The transport of charged particles in this structure is usually performed by Dirac equation (which is the relativistic counterpart of the Schrödinger equation). Due to the unusual properties of graphene -at room temperature, electrons moving in graphene behave as massless relativistic particles- physicists and compagnies are nowadays actively studying this material. Here, predicting how the material properties are affected by the uncertainties in the hexagonal lattice structure or in external potentials, is a major issue. Then, one can wonder how to combine multiscale UA schemes with some well-known UQ numerical methods (as stochastic Galerkin (SG) approaches) ?

4.1.3. Population dynamics

The main goal is to characterize how spatial propagation phenomena (diffusion, transport, advection, ...) affect the time evolution of the demography of a population. In collaboration with Y. Lagadeuc (ECOBIO, Rennes), this question has been studied for plankton. In this context, mathematical models have been proposed and it has been shown that the spatial dynamic (in this context, due to the marine current) which is fast compared to demographic scales, can strongly modify the demographic evolution of the plankton.
In collaboration with Ecole d'Agronomie de Rennes, a mathematical study on the demography of a parasite fungi of plants has been performed. In this context, the demography is specific: the fungi can proliferate through sexual reproduction or through parthenogenesis. This two ways of reproduction give rise mathematically to quadratic and linear growth rates with respect to the population variable. The demography is then coupled with transport (transport of fungi spore by wind). Here, the goal is characterize the propagation of the fungi population by finding travelling waves solutions which are well adapted to describe the evolution of invasive fronts. Moreover, this approach enables to recover with a good agreement realistic examples (infection of ash or banana tree) for which experimental data are available.
In these contexts, mathematical models are a powerful tool for biologists since measurements are very complicated to obtain and laboratory experiments hardly reproduce reality. The models derived are multiscale due to the nature of the underlying phenomena and the next step is to provide efficient numerical schemes.

MOKAPLAN Project-Team (section vide)

NACHOS Project-Team

4. Application Domains

4.1. Electromagnetic wave propagation

Electromagnetic devices are ubiquitous in present day technology. Indeed, electromagnetism has found and continues to find applications in a wide array of areas, encompassing both industrial and societal purposes. Applications of current interest include (among others) those related to communications (e.g transmission through optical fiber lines), to biomedical devices (e.g microwave imaging, micro-antenna design for telemedecine, etc.), to circuit or magnetic storage design (electromagnetic compatibility, hard disc operation), to geophysical prospecting, and to non-destructive evaluation (e.g crack detection), to name but just a few. Equally notable and motivating are applications in defence which include the design of military hardware with decreased signatures, automatic target recognition (e.g bunkers, mines and buried ordnance, etc.) propagation effects on communication and radar systems, etc. Although the principles of electromagnetics are well understood, their application to practical configurations of current interest, such as those that arise in connection with the examples above, is significantly complicated and far beyond manual calculation in all but the simplest cases. These complications typically arise from the geometrical characteristics of the propagation medium (irregular shapes, geometrical singularities), the physical characteristics of the propagation medium (heterogeneity, physical dispersion and dissipation) and the characteristics of the sources (wires, etc.).

Although many of the above-mentioned application contexts can potentially benefit from numerical modeling studies, the team currently concentrates its efforts on two physical situations.

4.1.1. Microwave interaction with biological tissues

Two main reasons motivate our commitment to consider this type of problem for the application of the numerical methodologies developed in the NACHOS project-team:

- First, from the numerical modeling point of view, the interaction between electromagnetic waves and biological tissues exhibit the three sources of complexity identified previously and are thus particularly challenging for pushing one step forward the state-of-the art of numerical methods for computational electromagnetics. The propagation media is strongly heterogeneous and the electromagnetic characteristics of the tissues are frequency dependent. Interfaces between tissues have rather complicated shapes that cannot be accurately discretized using cartesian meshes. Finally, the source of the signal often takes the form of a complicated device (e.g a mobile phone or an antenna array).
- Second, the study of the interaction between electromagnetic waves and living tissues is of interest to several applications of societal relevance such as the assessment of potential adverse effects of electromagnetic fields or the utilization of electromagnetic waves for therapeutic or diagnostic purposes. It is widely recognized nowadays that numerical modeling and computer simulation of electromagnetic wave propagation in biological tissues is a mandatory path for improving the scientific knowledge of the complex physical mechanisms that characterize these applications.

Despite the high complexity both in terms of heterogeneity and geometrical features of tissues, the great majority of numerical studies so far have been conducted using variants of the widely known FDTD method due to Yee [48]. In this method, the whole computational domain is discretized using a structured (cartesian) grid. Due to the possible straightforward implementation of the algorithm and the availability of computational power, FDTD is currently the leading method for numerical assessment of human exposure to electromagnetic waves. However, limitations are still seen, due to the rather difficult departure from the commonly used rectilinear grid and cell size limitations regarding very detailed structures of human tissues. In this context, the general objective of the contributions of the NACHOS project-team is to demonstrate the benefits of high order unstructured mesh based Maxwell solvers for a realistic numerical modeling of the interaction of electromagnetic waves and biological tissues with emphasis on applications related to numerical dosimetry.

Since the creation of the team, our works on this topic have mainly been focussed on the study of the exposure of humans to radiations from mobile phones or wireless communication systems (see Fig. 1). This activity has been conducted in close collaboration with the team of Joe Wiart at Orange Labs/Whist Laboratory (http://whist.institut-telecom.fr/en/index.html) (formerly, France Telecom Research & Development) in Issy-les-Moulineaux [8].

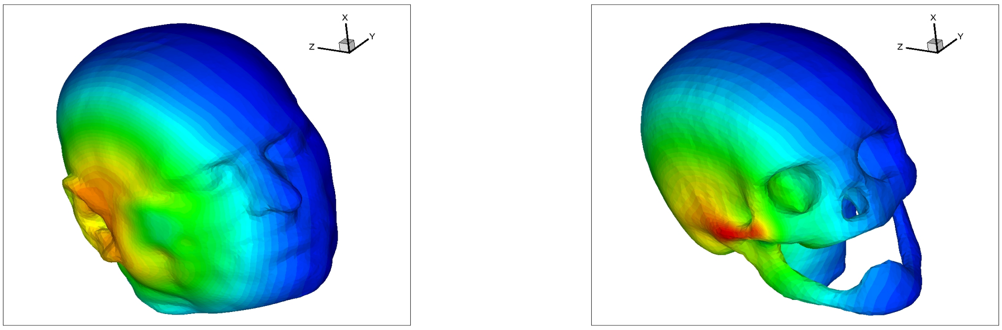


Figure 1. Exposure of head tissues to an electromagnetic wave emitted by a localized source. Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

4.1.2. Light-matter interaction on the nanoscale

Nanostructuring of materials has opened up a number of new possibilities for manipulating and enhancing light-matter interactions, thereby improving fundamental device properties. Low-dimensional semiconductors, like quantum dots, enable one to catch the electrons and control the electronic properties of a material, while photonic crystal structures allow to synthesize the electromagnetic properties. These technologies may, e.g., be employed to make smaller and better lasers, sources that generate only one photon at a time, for applications in quantum information technology, or miniature sensors with high sensitivity. The incorporation of metallic structures into the medium add further possibilities for manipulating the propagation of electromagnetic waves. In particular, this allows subwavelength localisation of the electromagnetic field and, by subwavelength structuring of the material, novel effects like negative refraction, e.g. enabling super lenses, may be realized. Nanophotonics is the recently emerged, but already well defined, field of science and technology aimed at establishing and using the peculiar properties of light and light-matter interaction in various nanostructures. Nanophotonics includes all the phenomena that are used in optical sciences for the development of optical devices. Therefore, nanophotonics finds numerous applications such as in optical microscopy, the design of optical switches and electromagnetic chips circuits, transistor filaments, etc. Because of its numerous scientific and technological applications (e.g. in relation to telecommunication, energy production and biomedicine), nanophotonics represents an active field of research increasingly relying on numerical modeling beside experimental studies.

Plasmonics is a related field to nanophotonics. Metallic nanostructures whose optical scattering is dominated by the response of the conduction electrons are considered as plasmomic media. If the structure presents an interface with e.g. a dielectric with a positive permittivity, collective oscillations of surface electrons create surface-plasmons-polaritons (SPPs) that propagate along the interface. SPPs are guided along metal-dielectric interfaces much in the same way light can be guided by an optical fiber, with the unique characteristic of subwavelength-scale confinement perpendicular to the interface. Nanofabricated systems that exploit SPPs offer fascinating opportunities for crafting and controlling the propagation of light in matter. In particular, SPPs can be used to channel light efficiently into nanometer-scale volumes, leading to direct modification of mode dispersion properties (substantially shrinking the wavelength of light and the speed of light pulses for example), as well as huge field enhancements suitable for enabling strong interactions with non-linear materials. The resulting enhanced sensitivity of light to external parameters (for example, an applied electric field or the dielectric constant of an adsorbed molecular layer) shows great promise for applications in sensing and switching. In particular, very promising applications are foreseen in the medical domain [40]- [49].

Numerical modeling of electromagnetic wave propagation in interaction with metallic nanostructures at optical frequencies requires to solve the system of Maxwell equations coupled to appropriate models of physical dispersion in the metal, such as the Drude and Drude-Lorentz models. Here again, the FDTD method is a widely used approach for solving the resulting system of PDEs [45]. However, for nanophotonic applications, the space and time scales, in addition to the geometrical characteristics of the considered nanostructures (or structured layouts of the latter), are particularly challenging for an accurate and efficient application of the FDTD method. Recently, unstructured mesh based methods have been developed and have demonstrated their potentialities for being considered as viable alternatives to the FDTD method [43]- [44]- [38]. Since the end of 2012, nanophotonics/plasmonics is increasingly becoming a focused application domain in the research activities of the team in close collaboration with physicists from CNRS laboratories, and also with researchers from international institutions.

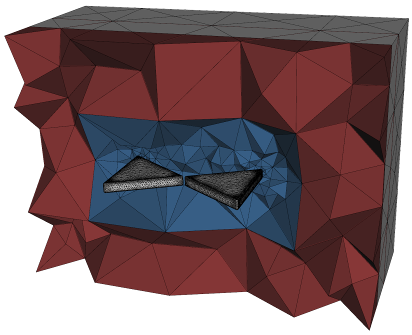


Figure 2. Simulation of the field enhancement at the tip of a gold bowtie nanoantenna (PhD thesis of Jonathan Viquerat).

4.2. Elastodynamic wave propagation

Elastic wave propagation in interaction with solids are encountered in a lot of scientific and engineering contexts. One typical example is geoseismic wave propagation for earthquake dynamics or resource prospection.

4.2.1. Earthquake dynamics

To understand the basic science of earthquakes and to help engineers better prepare for such an event, scientists want to identify which regions are likely to experience the most intense shaking, particularly in populated sediment-filled basins. This understanding can be used to improve buildings in high hazard areas and to help engineers design safer structures, potentially saving lives and property. In the absence of deterministic earthquake prediction, forecasting of earthquake ground motion based on simulation of scenarios is one of the most promising tools to mitigate earthquake related hazard. This requires intense modeling that meets the spatial and temporal resolution scales of the continuously increasing density and resolution of the seismic instrumentation, which record dynamic shaking at the surface, as well as of the basin models. Another important issue is to improve the physical understanding of the earthquake rupture processes and seismic wave propagation. Large-scale simulations of earthquake rupture dynamics and wave propagation are currently the only means to investigate these multiscale physics together with data assimilation and inversion. High resolution models are also required to develop and assess fast operational analysis tools for real time seismology and early warning systems.

Numerical methods for the propagation of seismic waves have been studied for many years. Most of existing numerical software rely on finite difference type methods. Among the most popular schemes, one can cite the staggered grid finite difference scheme proposed by Virieux [46] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by Yee [48] for the solution of the Maxwell equations. Many improvements of this method have been proposed, in particular, higher order schemes in space or rotated staggered-grids allowing strong fluctuations of the elastic parameters. Despite these improvements, the use of cartesian grids is a limitation for such numerical methods especially when it is necessary to incorporate surface topography or curved interface. Moreover, in presence of a non planar topography, the free surface condition needs very fine grids (about 60 points by minimal Rayleigh wavelength) to be approximated. In this context, our objective is to develop high order unstructured mesh based methods for the numerical solution of the system of elastodynamic equations for elastic media in a first step, and then to extend these methods to a more accurate treatment of the heterogeneities of the medium or to more complex propagation materials such as viscoelastic media which take into account the intrinsic attenuation. Initially, the team has considered in detail the necessary methodological developments for the large-scale simulation of earthquake dynamics [1]. More recently, the team has collaborated with CETE Méditerranée which is a regional technical and engineering centre whose activities are concerned with seismic hazard assessment studies, and IFSTTAR (https://www.ifsttar.fr/en/welcome/) which is the French institute of science and technology for transport, development and networks, conducting research studies on control over aging, risks and nuisances.

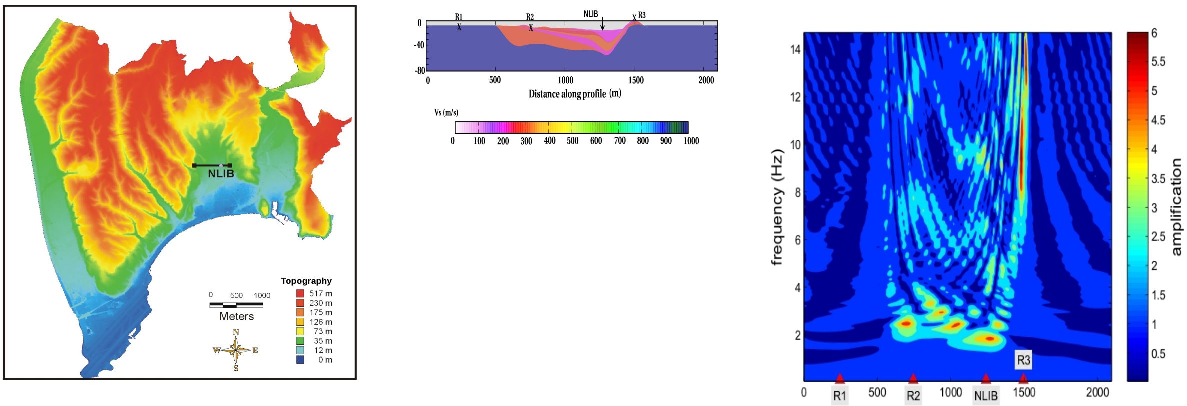


Figure 3. Propagation of a plane wave in a heterogeneous model of Nice area (provided by CETE Méditerranée). Left figure: topography of Nice and location of the cross-section used for numerical simulations (black line). Middle figure: S-wave velocity distribution along the cross-section in the Nice basin. Right figure: transfer functions (amplification) for a vertically incident plane wave ; receivers every 5 m at the surface. This numerical simulation was performed using a numerical method for the solution of the elastodynamics equations coupled to a Generalized Maxwell Body (GMB) model of viscoelasticity (PhD thesis of Fabien Peyrusse).

4.2.2. Seismic exploration

This application topic is considered in close collaboration with the MAGIQUE-3D project-team at Inria Bordeaux - Sud-Ouest which is coordinating the Depth Imaging Partnership (DIP -http://dip.inria.fr) between Inria and TOTAL. The research program of DIP includes different aspects of the modeling and numerical simulation of sesimic wave propagation that must be considered to construct an efficient software suites for producing accurate images of the subsurface. Our common objective with the MAGIQUE-3D project-team is to design high order unstructured mesh based methods for the numerical solution of the system of elastodynamic equations in the time-domain and in the frequency-domain, that will be used as forward modelers in appropriate inversion procedures.

NANO-D Project-Team (section vide)

RAPSODI Project-Team

4. Application Domains

4.1. Porous media flows

Porous media flows are of great interest in many contexts, like, e.g., oil engineering, water resource management, nuclear waste repository management, or carbon dioxyde sequestration. We refer to [57], [56] for an extensive discussion on porous media flow models.

From a mathematical point of view, the transport of complex fluids in porous media often leads to possibly degenerate parabolic conservation laws. The porous rocks can be highly heterogeneous and anisotropic. Moreover, the grids on which one intends to solve numerically the problems are prescribed by the geological data, and might be non-conformal with cells of various shapes. Therefore, the schemes used for simulating such complex flows must be particularly robust.

4.2. Corrosion and concrete carbonation

The team is interested in the theoretical and numerical analysis of mathematical models describing degradation of materials as concrete carbonation and corrosion. The study of such models is an important environmental and industrial issue. Atmospheric carbonation degrades reinforced concretes and limits the lifetime of civil engineering structures. Corrosion phenomena issues occur for instance in the reliability of nuclear power plants and the nuclear waste repository. The study of the long time evolution of these phenomena is of course fundamental in order to predict the lifetime of the structures.

From a mathematical point of view, the modeling of concrete carbonation (see [51]) as the modeling of corrosion in an underground repository (DPCM model developed by Bataillon *et al.* [55]) lead to systems of PDEs posed on moving domains. The coupling between convection-diffusion-reaction equations and moving boundary equations leads to challenging mathematical questions.

4.3. Complex fluid flows

The team is interested in some numerical methods for the simulation of systems of PDEs describing complex flows, like for instance, mixture flows, granular gases, rarefied gases, or quantum fluids.

Variable-density, low-Mach flows have been widely studied in the recent literature because of their applicability in various phenomena such as flows in high-temperature gas reactors, meteorological flows, flows with convective and/or conductive heat transfer or combustion processes. In such cases, the resolution of the full compressible Navier–Stokes system is not adapted, because of the sound waves speed. The Boussinesq incompressible model is not a better alternative for such low-speed phenomena, because the compressibility effects can not be totally cancelled due to large variations of temperature and density. Consequently, some models have been formally derived, leading to the filtering of the acoustic waves by the use of some formal asymptotic expansions and two families of methods have been developed in the literature in order to compute these flows. We are interested in particular in the so-called pressure-based methods which are more robust than density-based solvers, although their range of validity is in general more limited.

Kinetic theory of molecular gases models a gas as a system of elastically colliding spheres, conserving mechanical energy during impact. Once initialized, it takes a molecular gas not more than few collisions per particle to relax to its equilibrium state, characterized by a Maxwellian velocity distribution and a certain homogeneous density (in the absence of external forces). A granular gas is a system of dissipatively colliding, macroscopic particles (grains). This slight change in the microscopic dynamics (converting energy into heat) cause drastic changes in the behavior of the gas: granular gases are open systems, which exhibits self-organized spatio-temporal cluster formations, and has no equilibrium distribution. They can be used to model silos, avalanches, pollen or planetary rings.

The quantum models can be used to describe superfluids, quantum semiconductors, weakly interacting Bose gases or quantum trajectories of Bohmian mechanics. They have attracted considerable attention in the last decades, due in particular to the development of the nanotechnology applications. To describe quantum phenomena, there exists a large variety of models. In particular there exist three different levels of description: microscopic, mesoscopic and macroscopic. The quantum Navier–Stokes equations deal with a macroscopic description in which the quantum effects are taken into account through a third order term called the quantum Bohm potential. This Bohm potential arises from the fluid dynamical formulation of the single-state Schrödinger equation. The non-locality of quantum mechanics is approximated by the fact that the equations of state do not only depend on the particle density but also on its gradient. These equations were employed to model field emissions from metals and steady-state tunneling in metal- insulator- metal structures and to simulate ultra-small semiconductor devices.

4.4. Stratigraphy

The knowledge of the geology is a prerequisite before simulating flows within the subsoil. Numerical simulations of the geological history thanks to stratigraphy numerical codes allow to complete the knowledge of the geology where experimental data are lacking. Stratigraphic models consist in a description of the erosion and sedimentation phenomena at geological scales.

The characteristic time scales for the sediments are much larger than the characteristic time scales for the water in the river. However, the (time-averaged) water flux plays a crucial role in the evolution of the stratigraphy. Therefore, defining appropriate models that take the coupling between the rivers and the sediments into account is fundamental and challenging. Once the models are at hand, efficient numerical methods must be developed.

4.5. Low-frequency electromagnetism

Numerical simulation is nowadays an essential tool in order to design electromagnetic systems, by estimating the electromagnetic fields generated in a wide variety of devices. An important challenge for many applications is to quantify the intensity of the electric field induced in a conductor by a current generated in its neighborhood. In the low-frequency regime, we can for example quote the study of the impact on the human body of a high-tension line or, for higher frequencies, the one of a smartphone. But the ability to simulate accurately some electromagnetic fields is also very useful for non-destructive control, in the context of the maintenance of nuclear power stations for example. The development of efficient numerical tools, among which *a posteriori* error estimators, is consequently necessary to reach a high precision of calculation in order to provide estimations as reliable as possible.

CAGE Project-Team

4. Application Domains

4.1. First axis: Geometry of vision

A suggestive application of sub-Riemannian geometry and in particular of hypoelliptic diffusion comes from a model of geometry of vision describing the functional architecture of the primary visual cortex V1. In 1958, Hubel and Wiesel (Nobel in 1981) observed that the visual cortex V1 is endowed with the so-called **pinwheel structure**, characterized by neurons grouped into orientation columns, that are sensible both to positions and directions [109]. The mathematical rephrasing of this discovery is that the visual cortex lifts an image from $\mathbf{R}^2$ into the bundle of directions of the plane [95], [136], [138], [108].

A simplified version of the model can be described as follows: neurons of V1 are grouped into orientation columns, each of them being sensitive to visual stimuli at a given point of the retina and for a given direction on it. The retina is modeled by the real plane, i.e., each point is represented by a pair $(x, y) \in \mathbb{R}^2$, while the directions at a given point are modeled by the projective line, i.e. an element θ of the projective line P^1. Hence, the primary visual cortex V1 is modeled by the so called projective tangent bundle $\mathrm{PTR}^2 = \mathbf{R}^2 \times \mathbf{P}^1$. From a neurological point of view, orientation columns are in turn grouped into hypercolumns, each of them being sensitive to stimuli at a given point (x, y) with any direction.

Orientation columns are connected between them in two different ways. The first kind of connections are the vertical (inhibitory) ones, which connect orientation columns belonging to the same hypercolumn and sensible to similar directions. The second kind of connections are the horizontal (excitatory) connections, which connect neurons belonging to different (but not too far) hypercolumns and sensible to the same directions. The resulting metric structure is sub-Riemannian and the model obtained in this way provides a convincing explanation in terms of sub-Riemannian geodesics of gestalt phenomena such as Kanizsa illusory contours.

The sub-Riemannian model for image representation of V1 has a great potential of yielding powerful bio-inspired image processing algorithms [102], [88]. Image inpainting, for instance, can be implemented by reconstructing an incomplete image by activating orientation columns in the missing regions in accordance with sub-Riemannian non-isotropic constraints. The process intrinsically defines an hypoelliptic heat equation on PTR^2 which can be integrated numerically using non-commutative Fourier analysis on a suitable semidiscretization of the group of roto-translations of the plane [86].

We have been working on the model and its software implementation since 2012. This work has been supported by several project, as the ERC starting grant GeCoMethods and the ERC Proof of Concept ARTIV1 of U. Boscain, and the ANR GCM.

A parallel approach that we will pursue and combine with this first one is based on **pattern matching in the group of diffeomorphisms**. We want to extend this approach, already explored in the Riemannian setting [151], [126], to the general sub-Riemannian framework. The paradigm of the approach is the following: consider a distortable object, more or less rigid, discretized into a certain number of points. One may track its distortion by considering the paths drawn by these points. One would however like to know how the object itself (and not its discretized version) has been distorted. The study in [151], [126] shed light on the importance of Riemannian geometry in this kind of problem. In particular, they study the Riemannian submersion obtained by making the group of diffeomorphisms act transitively on the manifold formed by the points of the discretization, minimizing a certain energy so as to take into account the whole object. Settled as such, the problem is Riemannian, but if one considers objects involving connections, or submitted to nonholonomic constraints, like in medical imaging where one tracks the motions of organs, then one comes up with a sub-Riemannian problem. The transitive group is then far bigger, and the aim is to lift curves submitted to these nonholonomic constraints into curves in the set of diffeomorphisms satisfying the corresponding constraints, in a unique way and minimizing an energy (giving rise to a sub-Riemannian structure).

4.2. Second axis: Quantum control

The goal of quantum control is to design efficient protocols for tuning the occupation probabilities of the energy levels of a system. This task is crucial in atomic and molecular physics, with applications ranging from photochemistry to nuclear magnetic resonance and quantum computing. A quantum system may be controlled by exciting it with one or several external fields, such as magnetic or electric fields. The goal of quantum control theory is to adapt the tools originally developed by control theory and to develop new specific strategies that tackle and exploit the features of quantum dynamics (probabilistic nature of wavefunctions and density operators, measure and wavefunction collapse, decoherence, ...). A rich variety of relevant models for controlled quantum dynamics exist, encompassing low-dimensional models (e.g., single-spin systems) and PDEs alike, with deterministic and stochastic components, making it a rich and exciting area of research in control theory.

The controllability of quantum system is a well-established topic when the state space is finite-dimensional [100], thanks to general controllability methods for left-invariant control systems on compact Lie groups [90], [111]. When the state space is infinite-dimensional, it is known that in general the bilinear Schrödinger equation is not exactly controllable [154]. Nevertheless, weaker controllability properties, such as approximate controllability or controllability between eigenstates of the internal Hamiltonian (which are the most relevant physical states), may hold. In certain cases, when the state space is a function space on a 1D manifold, some rather precise description of the set of reachable states has been provided [75]. A similar description for higher-dimensional manifolds seems intractable and at the moment only approximate controllability results are available [127], [134], [112]. The most widely applicable tests for controllability of quantum systems in infinite-dimensional Hilbert spaces are based on the **Lie–Galerkin technique** [94], [83], [84]. They allow, in particular, to show that the controllability property is generic among this class of systems [124].

A family of algorithms which are specific to quantum systems are those based on adiabatic evolution [158], [157], [115]. The basic principle of adiabatic control is that the flow of a slowly varying Hamiltonian can be approximated (up to a phase factor) by a quasi-static evolution, with a precision proportional to the velocity of variation of the Hamiltonian. The advantage of the **adiabatic approach** is that it is constructive and produces control laws which are both smooth and robust to parameter uncertainty. The paradigm is based on the adiabatic perturbation theory developed in mathematical physics [81], [133], [150], where it plays an important role for understanding molecular dynamics. Approximation theory by adiabatic perturbation can be used to describe the evolution of the occupation probabilities of the energy levels of a slowly varying Hamiltonian. Results from the last 15 years, including those by members of our team [62], [87], have highlighted the effectiveness of control techniques based on adiabatic path following.

4.3. Third axis: Stability and uncertain dynamics

Switched and hybrid systems constitute a broad framework for the description of the heterogeneous aspects of systems in which continuous dynamics (typically pertaining to physical quantities) interact with discrete/logical components. The development of the switched and hybrid paradigm has been motivated by a broad range of applications, including automotive and transportation industry [142], energy management [135] and congestion control [125].

Even if both controllability [146] and observability [113] of switched and hybrid systems have attracted much research efforts, the central role in their study is played by the problem of stability and stabilizability. The goal is to determine whether a dynamical or a control system whose evolution is influenced by a time-dependent signal is uniformly stable or can be uniformly stabilized [118], [147]. Uniformity is considered with respect to all signals in a given class. Stability of switched systems lead to several interesting phenomena. For example, even when all the subsystems corresponding to a constant switching law are exponentially stable, the switched systems may have divergent trajectories for certain switching signals [117]. This fact illustrates the fact that stability of switched systems depends not only on the dynamics of each subsystem but also on the properties of the class of switching signals which is considered.

The most common class of switching signals which has been considered in the literature is made of all piecewise constant signals. In this case uniform stability of the system is equivalent to the existence of a common quadratic Lyapunov function [128]. Moreover, provided that the system has finitely many modes, the Lyapunov function can be taken polyhedral or polynomial [78], [79], [101]. A special role in the switched control literature has been played by common quadratic Lyapunov functions, since their existence can be tested rather efficiently (see the surveys [120], [141] and the references therein). It is known, however, that the existence of a common quadratic Lyapunov function is not necessary for the global uniform exponential stability of a linear switched system with finitely many modes. Moreover, there exists no uniform upper bound on the minimal degree of a common polynomial Lyapunov function [123]. More refined tools rely on multiple and non-monotone Lyapunov functions [89]. Let us also mention linear switched systems technics based on the analysis of the Lie algebra generated by the matrices corresponding to the modes of the system [65].

For systems evolving in the plane, more geometrical tests apply, and yield a complete characterization of the stability [82], [71]. Such a geometric approach also yields sufficient conditions for uniform stability in the linear planar case [85].

In many situations, it is interesting for modeling purposes to specify the features of the switched system by introducing **constrained switching rules**. A typical constraint is that each mode is activated for at least a fixed minimal amount of time, called the dwell-time. Switching rules can also be imposed, for instance, by a timed automata. When constraints apply, the common Lyapunov function approach becomes conservative and new tools have to be developed to give more detailed characterizations of stable and unstable systems.

Our approach to constrained switching is based on the idea of relating the analytical properties of the classes of constrained switching laws (shift-invariance, compactness, closure under concatenation, ...) to the stability behavior of the corresponding switched systems. One can introduce **probabilistic uncertainties** by endowing the classes of admissible signals with suitable probability measures. One then looks at the corresponding Lyapunov exponents, whose existence is established by the multiplicative ergodic theorem. The interest of this approach is that probabilistic stability analysis filters out highly 'exceptional' worst-case trajectories. Although less explicitly characterized from a dynamical viewpoint than its deterministic counterpart, the probabilistic notion of uniform exponential stability can be studied using several reformulations of Lyapunov exponents proposed in the literature [76], [96], [155].

4.4. Joint theoretical core

The theoretical questions raised by the different applicative area will be pooled in a research axis on the transversal aspects of geometric control theory and sub-Riemannian structures.

We recall that sub-Riemannian geometry is a generalization of Riemannian geometry, whose birth dates back to Carathéodory's seminal paper on the foundations of Carnot thermodynamics [92], followed by E. Cartan's address at the International Congress of Mathematicians in Bologna [93]. In the last twenty years, sub-Riemannian geometry has emerged as an independent research domain, with a variety of motivations and ramifications in several parts of pure and applied mathematics. Let us mention geometric analysis, geometric measure theory, stochastic calculus and evolution equations together with applications in mechanics and optimal control (motion planning, robotics, nonholonomic mechanics, quantum control) [60], [61].

One of the main open problems in sub-Riemannian geometry concerns the regularity of length-minimizers [63], [130]. Length-minimizers are solutions to a variational problem with constraints and satisfy a first-order necessary condition resulting from the Pontryagin Maximum Principle (PMP). Solutions of the PMP are either *normal* or *abnormal*. Normal length-minimizer are well-known to be smooth, i.e., C^∞, as it follows by the Hamiltonian nature of the PMP. The question of regularity is then reduced to abnormal length-minimizers. If the sub-Riemannian structure has step 2, then abnormal length-minimizers can be excluded and thus every length-minimizer is smooth. For step 3 structures, the situation is already more complicated and smoothness of length-minimizers is known only for Carnot groups [114], [149]. The question of regularity of length-minimizers is not restricted to the smoothness in the C^∞ sense. A recent result prove that length-minimizers, for sub-Riemannian structures of any step, cannot have corner-like singularities [107]. When the sub-Riemannian structure is analytic, more is known on the size of the set of points where a length-minimizer can lose analyticity [148], regardless of the rank and of the step of the distribution.

An interesting set of recent results in sub-Riemannian geometry concerns the extension to such a setting of the Riemannian notion of sectional curvature. The curvature operator can be introduced in terms of the symplectic invariants of the Jacobi curve [67], [116], [64], a curve in the Lagrange Grassmannian related to the linearization of the Hamiltonian flow. Alternative approaches to curvatures in metric spaces are based either on the associated heat equation and the generalization of the curvature-dimension inequality [72], [73] or on optimal transport and the generalization of Ricci curvature [145], [144], [122], [69].

COMMANDS Project-Team

4. Application Domains

4.1. Fuel saving by optimizing airplanes trajectories

We have a collaboration with the startup Safety Line on the optimization of trajectories for civil aircrafts. Key points include the reliable identification of the plane parameters (aerodynamic and thrust models) using data from the flight recorders, and the robust trajectory optimization of the climbing and cruise phases. We use both local (quasi-Newton interior-point algorithms) and global optimization tools (dynamic programming). The local method for the climb phase is in production and has been used for several hundreds of actual plane flights.

4.2. Hybrid vehicles

We have a collaboration with IFPEN on the energy management for hybrid vehicles. A significant direction is the analysis and classification of traffic data. More specifically, we focus on the traffic probability distribution in the (speed,torque) plane, with a time / space subdivision (road segments and timeframes).

4.3. Biological systems

2018 was the last year of IPL Algae in Silico in which we tackled the optimization of photobioreactors in turbid conditions. Our participation to IPL Cosy was strenghtened through the co-supervision of the PhD of E. Weill with team Lifeware (Inria and Pasteur), starting from september 2018, and focused on the oprimization of heterogenous populations of micro-organisms.

DISCO Project-Team

4. Application Domains

4.1. Analysis and Control of life sciences systems

The team is involved in life sciences applications. The two main lines are the analysis of bioreactors models and the modeling of cell dynamics in Acute Myeloblastic Leukemias (AML) in collaboration with St Antoine Hospital in Paris. A recent new subject is the modelling of Dengue epidemics.

4.2. Energy Management

The team is interested in Energy management and considers optimization and control problems in energy networks.

FACTAS Team

4. Application Domains

4.1. Introduction

Application domains are naturally linked to the problems described in Sections 3.2.1 and 3.2.2 . By and large, they split into a systems-and-circuits part and an inverse-source-and-boundary-problems part, united under a common umbrella of function-theoretic techniques as described in Section 3.3 .

4.2. Inverse magnetization problems

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

Generally speaking, inverse potential problems, similar to the one appearing in Section 4.3 , occur naturally in connection with systems governed by Maxwell's equation in the quasi-static approximation regime. In particular, they arise in magnetic reconstruction issues. A specific application is to geophysics, which led us to form the Inria Associate Team IMPINGE (Inverse Magnetization Problems IN GEosciences) together with MIT and Vanderbilt University. A recent collaboration with Cerege (CNRS, Aix-en-Provence), in the framework of the ANR-project MagLune, completes this picture, see Sections 6.1.2 , 8.2.1 .

To set up the context, recall that the Earth's geomagnetic field is generated by convection of the liquid metallic core (geodynamo) and that rocks become magnetized by the ambient field as they are formed or after subsequent alteration. Their remanent magnetization provides records of past variations of the geodynamo, which is used to study important processes in Earth sciences like motion of tectonic plates and geomagnetic reversals. Rocks from Mars, the Moon, and asteroids also contain remanent magnetization which indicates the past presence of core dynamos. Magnetization in meteorites may even record fields produced by the young sun and the protoplanetary disk which may have played a key role in solar system formation.

For a long time, paleomagnetic techniques were only capable of analyzing bulk samples and compute their net magnetic moment. The development of SQUID microscopes has recently extended the spatial resolution to sub-millimeter scales, raising new physical and algorithmic challenges. The associate team IMPINGE aims at tackling them, experimenting with the SQUID microscope set up in the Paleomagnetism Laboratory of the department of Earth, Atmospheric and Planetary Sciences at MIT. Typically, pieces of rock are sanded down to a thin slab, and the magnetization has to be recovered from the field measured on a planar region at small distance from the slab.

Mathematically speaking, both inverse source problems for EEG from Section 4.3 and inverse magnetization problems described presently amount to recover the (3-D valued) quantity m (primary current density in case of the brain or magnetization in case of a thin slab of rock) from measurements of the potential:

$$\int_{\Omega} \frac{\operatorname{div} m(x')\, dx'}{|x-x'|}\,, \tag{2}$$

outside the volume Ω of the object. The difference is that the distribution m is located in a volume in the case of EEG, and on a plane in the case of rock magnetization. This results in quite different identifiability properties, see [35] and Section 6.1.1 , but the two situations share a substantial mathematical common core.

Another timely instance of inverse magnetization problems lies with geomagnetism. Satellites orbiting around the Earth measure the magnetic field at many points, and nowadays it is a challenge to extract global information from those measurements. In collaboration with C. Gerhards (since September with the Geomathematics and Geoinformatics Group, Technische Universität Bergakademie Freiberg, Germany; until then, Univ. of Vienna, Austria), we started to work on the problem of separating the magnetic field due to the magnetization of the globe's crust from the magnetic field due to convection in the liquid metallic core. The techniques involved are variants, in a spherical context, from those developed within the IMPINGE associate team for paleomagnetism, see Section 6.1.1 .

4.3. Inverse source problems in EEG

Participants: Laurent Baratchart, Juliette Leblond, Jean-Paul Marmorat.

This work is conducted in collaboration with Maureen Clerc and Théo Papadopoulo from the team Athena (Inria Sophia).

Solving overdetermined Cauchy problems for the Laplace equation on a spherical layer (in 3-D) in order to extrapolate incomplete data (see Section 3.2.1) is a necessary ingredient of the team's approach to inverse source problems, in particular for applications to EEG, see [8]. Indeed, the latter involves propagating the initial conditions through several layers of different conductivities, from the boundary shell down to the center of the domain where the singularities (*i.e.* the sources) lie. Once propagated to the innermost sphere, it turns out that traces of the boundary data on 2-D cross sections coincide with analytic functions with branched singularities in the slicing plane [7], [40]. The singularities are related to the actual location of the sources, namely their moduli reach in turn a maximum when the plane contains one of the sources. Hence we are back to the 2-D framework of Section 3.3.3 , and recovering these singularities can be performed *via* best rational approximation. The goal is to produce a fast and sufficiently accurate initial guess on the number and location of the sources in order to run heavier descent algorithms on the direct problem, which are more precise but computationally costly and often fail to converge if not properly initialized. Our belief is that such a localization process can add a geometric, valuable piece of information to the standard temporal analysis of EEG signal records.

Numerical experiments obtained with our software FindSources3D give very good results on simulated data and we are now engaged in the process of handling real experimental data (see Sections 3.4.2 and 6.1), in collaboration with our partners at INS, hospital la Timone, Marseille.

4.4. Identification and design of microwave devices

Participants: Laurent Baratchart, Sylvain Chevillard, Jean-Paul Marmorat, Martine Olivi, Fabien Seyfert.

This is joint work with Stéphane Bila (XLIM, Limoges).

One of the best training grounds for function-theoretic applications by the team is the identification and design of physical systems whose performance is assessed frequency-wise. This is the case of electromagnetic resonant systems which are of common use in telecommunications.

In space telecommunications (satellite transmissions), constraints specific to on-board technology lead to the use of filters with resonant cavities in the microwave range. These filters serve multiplexing purposes (before or after amplification), and consist of a sequence of cylindrical hollow bodies, magnetically coupled by irises (orthogonal double slits). The electromagnetic wave that traverses the cavities satisfies the Maxwell equations, forcing the tangent electrical field along the body of the cavity to be zero. A deeper study of the Helmholtz equation states that an essentially discrete set of wave vectors is selected. In the considered range of frequency, the electrical field in each cavity can be decomposed along two orthogonal modes, perpendicular to the axis of the cavity (other modes are far off in the frequency domain, and their influence can be neglected).

Each cavity (see Figure 1) has three screws, horizontal, vertical and midway (horizontal and vertical are two arbitrary directions, the third direction makes an angle of 45 or 135 degrees, the easy case is when all cavities show the same orientation, and when the directions of the irises are the same, as well as the input and output slits). Since screws are conductors, they behave as capacitors; besides, the electrical field on the surface has to be zero, which modifies the boundary conditions of one of the two modes (for the other mode, the electrical field is zero hence it is not influenced by the screw), the third screw acts as a coupling between the two modes. The effect of an iris is opposite to that of a screw: no condition is imposed on a hole, which results in a coupling between two horizontal (or two vertical) modes of adjacent cavities (in fact the iris is the union of two rectangles, the important parameter being their width). The design of a filter consists in finding the size of each cavity, and the width of each iris. Subsequently, the filter can be constructed and tuned by adjusting the screws. Finally, the screws are glued once a satisfactory response has been obtained. In what follows, we shall consider a typical example, a filter designed by the CNES in Toulouse, with four cavities near 11 GHz.

Figure 1. Picture of a 6-cavities dual mode filter. Each cavity (except the last one) has 3 screws to couple the modes within the cavity, so that 16 quantities must be optimized. Quantities such as the diameter and length of the cavities, or the width of the 11 slits are fixed during the design phase.

Near the resonance frequency, a good approximation to the Helmholtz equations is given by a second order differential equation. Thus, one obtains an electrical model of the filter as a sequence of electrically-coupled resonant circuits, each circuit being modeled by two resonators, one per mode, the resonance frequency of which represents the frequency of a mode, and whose resistance accounts for electric losses (surface currents) in the cavities.

This way, the filter can be seen as a quadripole, with two ports, when plugged onto a resistor at one end and fed with some potential at the other end. One is now interested in the power which is transmitted and reflected. This leads one to define a scattering matrix S, which may be considered as the transfer function of a stable causal linear dynamical system, with two inputs and two outputs. Its diagonal terms $S_{1,1}$, $S_{2,2}$ correspond to reflections at each port, while $S_{1,2}$, $S_{2,1}$ correspond to transmission. These functions can be measured at certain frequencies (on the imaginary axis). The matrix S is approximately rational of order 4 times the number of cavities (that is 16 in the example on Figure 2), and the key step consists in expressing the components of the equivalent electrical circuit as functions of the S_{ij} (since there are no formulas expressing the lengths of the screws in terms of parameters of this electrical model). This representation is also useful to analyze the numerical simulations of the Maxwell equations, and to check the quality of a design, in particular the absence of higher resonant modes.

In fact, resonance is not studied via the electrical model, but via a low-pass equivalent circuit obtained upon linearizing near the central frequency, which is no longer conjugate symmetric (*i.e.* the underlying system may no longer have real coefficients) but whose degree is divided by 2 (8 in the example).

In short, the strategy for identification is as follows:

- measuring the scattering matrix of the filter near the optimal frequency over twice the pass band (which is 80MHz in the example).
- Solving bounded extremal problems for the transmission and the reflection (the modulus of he response being respectively close to 0 and 1 outside the interval measurement, cf. Section 3.3.1) in order to get a models for the scattering matrix as an analytic matrix-valued function. This provides

us with a scattering matrix known to be close to a rational matrix of order roughly 1/4 of the number of data points.

- Approximating this scattering matrix by a true rational transfer-function of appropriate degree (8 in this example) via the Endymion or RARL2 software (cf. Section 3.3.2.2).
- A state space realization of S, viewed as a transfer function, can then be obtained, where additional symmetry constraints coming from the reciprocity law and possibly other physical features of the device have to be imposed.
- Finally one builds a realization of the approximant and looks for a change of variables that eliminates non-physical couplings. This is obtained by using algebraic-solvers and continuation algorithms on the group of orthogonal complex matrices (symmetry forces this type of transformation).

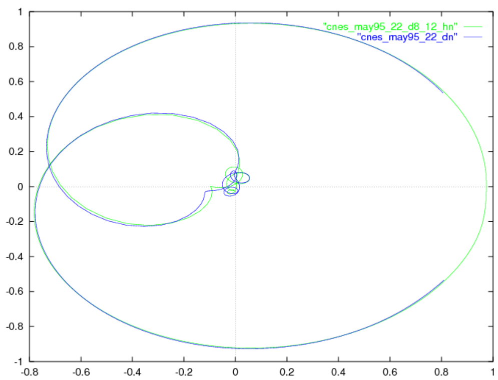


Figure 2. Nyquist Diagram. Rational approximation (degree 8) and data - S_{22}.

The final approximation is of high quality. This can be interpreted as a confirmation of the linearity assumption on the system: the relative L^2 error is less than 10^{-3}. This is illustrated by a reflection diagram (Figure 2). Non-physical couplings are less than 10^{-2}.

The above considerations are valid for a large class of filters. These developments have also been used for the design of non-symmetric filters, which are useful for the synthesis of repeating devices.

The team further investigates problems relative to the design of optimal responses for microwave devices. The resolution of a quasi-convex Zolotarev problems was proposed, in order to derive guaranteed optimal multi-band filter responses subject to modulus constraints [10]. This generalizes the classical single band design techniques based on Chebyshev polynomials and elliptic functions. The approach relies on the fact that the modulus of the scattering parameter $|S_{1,2}|$ admits a simple expression in terms of the filtering function $D = |S_{1,1}|/|S_{1,2}|$, namely

$$|S_{1,2}|^2 = \frac{1}{1 + D^2}.$$

The filtering function appears to be the ratio of two polynomials p_1/p_2, the numerator of the reflection and transmission scattering factors, that may be chosen freely. The denominator q is then obtained as the unique stable unitary polynomial solving the classical Feldtkeller spectral equation:

$$qq^* = p_1 p_1^* + p_2 p_2^*.$$

The relative simplicity of the derivation of a filter's response, under modulus constraints, owes much to the possibility of forgetting about Feldtkeller's equation and express all design constraints in terms of the filtering function. This no longer the case when considering the synthesis N-port devices for $N > 3$, like multiplexers, routers and power dividers, or when considering the synthesis of filters under matching conditions. The efficient derivation of multiplexers responses is the subject of recent investigation by Factas, using techniques based on constrained Nevanlinna-Pick interpolation (see Section 6.2).

Through contacts with CNES (Toulouse) and UPV (Bilbao), Apics got additionally involved in the design of amplifiers which, unlike filters, are active devices. A prominent issue here is stability. A twenty years back, it was not possible to simulate unstable responses, and only after building a device could one detect instability. The advent of so-called *harmonic balance* techniques, which compute steady state responses of linear elements in the frequency domain and look for a periodic state in the time domain of a network connecting these linear elements *via* static non-linearities made it possible to compute the harmonic response of a (possibly nonlinear and unstable) device [78]. This has had tremendous impact on design, and there is a growing demand for software analyzers. The team is also becoming active in this area.

In this connection, there are two types of stability involved. The first is stability of a fixed point around which the linearized transfer function accounts for small signal amplification. The second is stability of a limit cycle which is reached when the input signal is no longer small and truly nonlinear amplification is attained (*e.g.* because of saturation). Work by the team so far has been concerned with the first type of stability, and emphasis is put on defining and extracting the "unstable part" of the response, see Section 6.3 . The stability check for limit cycles is now under investigation.

I4S Project-Team (section vide)

MCTAO Project-Team

4. Application Domains

4.1. Aerospace Engineering

Space engineering is very demanding in terms of safe and high-performance control laws. It is therefore prone to fruitful industrial collaborations. McTAO now has an established expertise in space and celestial mechanics. Our collaborations with industry are mostly on orbit transfer problems with low-thrust propulsion. It can be orbit transfer to put a commercial satellite on station, in which case the dynamics are a Newtonian force field plus perturbations and the small control. There is also, currently, a renewed interest in low-thrust missions such as Lisa Pathfinder (ESA mission towards a Lagrange point of the Sun-Earth system) or BepiColombo (joint ESA-JAXA mission towards Mercury). Such missions look more like a controlled multibody system. In all cases the problem involves long orbit transfers, typically with many revolutions around the primary celestial body. When minimizing time, averaging techniques provide a good approximation. Another important criterion in practice is fuel consumption minimization (crucial because only a finite amount of fuel is onboard a satellite for all its “life”), which amounts to L^1-minimization. Both topics are studied by the team.

We have a steady relationships with CNES and Thales Alenia Space (Cannes), that have financed or co-financed 3 PhDs and 2 post-docs in the Sophia location of the team in the decade and are a source of inspiration even at the methodological level. Team members also have close connections with Airbus-Safran (Les Mureaux) on launchers.

Some of the authoritative papers in the field were written by team members, with an emphasis on the geometric analysis and on algorithms (coupling of shooting and continuation methods). There are also connections with peers more on the applied side, like D. Scheeres (Colorado Center for Astrodynamics Research at Boulder), the group of F. Bernelli (Politecnico Milano), and colleagues from U. Barcelona (A. Farrès, A. Jorba).

4.2. Magnetic resonance imaging (MRI)

The starting point of our interest in optimal control for quantum systems was a collaboration with physicist from ICB, University of Burgundy (Dominique Sugny), motivated by an ANR project where we worked on the control of molecular orientation in a dissipative environment using a laser field, and developed optimal control tools, combined with numerical simulations, to analyze the problem for Qubits. This was related to quantum computing rather than MRI.

Using this expertise and under the impulse of Prof. S. Glaser and his group (Chemistry, TU München), we investigated Nuclear Magnetic Resonance (NMR) for medical imaging (MRI), where the model is the Bloch equation describing the evolution of the magnetization vector controlled by a magnetic field, but in fine is a specific Qubit model without decoherence. We worked on, and brought strong contributions to, the contrast problem: typically, given two chemical substances that have an importance in medicine, like oxygenated and de-oxygenated blood, find the (time-dependent) magnetic field that will produce the highest difference in brightness between these two species on the image resulting from Nuclear Magnetic Resonance. This has immediate and important industrial applications in medical imaging. Our contacts are with the above mentioned physics academic labs, who are themselves in contact with major companies.

The team has produced and is producing important work on this problem. One may find a good overview in [50], a reference book has been published on the topic [54], a very complete numerical study comparing different optimization techniques was performed in [49]. We conduct this project in parallel with S. Glaser team, which validated experimentally the pertinence of the methods, the main achievement being the in vivo experiments realized at the Creatis team of Insa Lyon showing the interest to use optimal control methods implemented in modern softwares in MRI in order to produce a better image in a shorter time. A goal is to arrive to a cartography of the optimal contrast with respect to the relaxation parameters using LMI techniques and numerical simulations with the Hampath and Bocop code; note that the theoretical study is connected to the problem of understanding the behavior of the extremal solutions of a controlled pair of Bloch equations, and this is an ambitious task. Also, one of the difficulties to go from the obtained results, checkable on experiments, to practical control laws for production is to deal with magnetic field space inhomogeneities.

4.3. Swimming at low-Reynolds number

Following the historical reference for low Reynolds number locomotion [71], the study of the swimming strategies of micro-organisms is attracting increasing attention in the recent literature. This is both because of the intrinsic biological interest, and for the possible implications these studies may have on the design of bio-inspired artificial replicas reproducing the functionalities of biological systems. In the case of micro-swimmers, the surrounding fluid is dominated by the viscosity effects of the water and becomes reversible. In this regime, it turns out that the infinite dimensional dynamics of the fluid do not have to be retained as state variables, so that the dynamics of a micro-swimmer can be expressed by ordinary differential equations if its shape has a finite number of degrees of freedom. Assuming this finite dimension, and if the control is the rate of deformation, one obtains a control system that is linear (affine without drift) with respect to the controls, *i.e.* the optimal control problem with a quadratic cost defines a sub-Riemannian structure (see section 3.2). This is the case where the shape is "fully actuated", *i.e.* if all the variables describing the shape are angles, there is an actuator on each of these angles. For artificial micro-swimmers, this is usually unrealistic, hence (artificial) magneto-elastic micro-swimmers, that are magnetized in order to be deformed by an external magnetic field. In this case, the control functions are the external magnetic field.

In both cases, questions are controllability (straightforward in the fully actuated case), optimal control, possibly path planning. We collaborate with teams that have physical experiments for both.

- In collaboration with D. Takagi and M. Chyba (Univ of Hawaii), this approach is currently at the experimental level for copepod-like swimmer at the university of Hawaii: on the one hand, this zooplankton and its locomotion can be observed, and a robot micro swimmer mimicking a copepod has been constructed, but in fact large enough for direct actuation to be possible, and the low Reynolds number is achieved by using a more viscous fluid. This gives possibilities, through an inverse optimization problem, to determine what cost can be optimised by these crustaceans, see [5], [76], and to validate models on the robot.
- For magneto-elastic micro-robots, Y. El-Alaoui's PhD is co-advised with Stéphane Régnier from the robotics lab ISIR, Univ. Paris 6. Magneto-elastic micro-robots and their magnetic actuation are actually built at ISIR and the aim of the collaboration is to validate models and improve the existing control laws both in performance and in energy; of course, the micro scale does make things difficult.

The questions about optimality of periodic controls raised in Section 3.2 are related to these applications for periodic deformations, or strokes, play an important role in locomotion.

4.4. Stability of high frequency amplifiers

Nonlinear hyper-frequency amplifiers are ubiquitous in cell phone relays and many other devices. They must be as compact as possible, yielding complicated design. Computer Assisted Design tools are extensively used; for a given amplifier design, they provide frequency responses but fail to provide information of the stability of the response for each frequency. This stability is crucial for an unstable response will not be observed in practice; the actual device should not be built before stability is asserted. Predicting stability/instability from "simulations" in the Computer Assisted Design tool is of utmost importance (simulation between quotation marks because these simulations are in fact computations in the frequency domain).

Some techniques do exist (see a state of the art in [75]). They are pioneering but mildly reliable and not clearly mathematically grounded. Potential transfer is important.

This is the topic of an ongoing collaboration between McTAO and the project-team APICS. See results in section 7.15 .

NECS Project-Team

4. Application Domains

4.1. A large variety of application domains

Sensor and actuator networks are ubiquitous in modern world, thanks to the advent of cheap small devices endowed with communication and computation capabilities. Potential application domains for research in networked control and in distributed estimation are extremely various, and include the following examples.

- Intelligent buildings, where sensor information on CO_2 concentration, temperature, room occupancy, etc. can be used to control the heating, ventilation and air conditioning (HVAC) system under multi-objective considerations of comfort, air quality, and energy consumption.
- Smart grids: the operation of electrical networks is changing from a centralized optimization framework towards more distributed and adaptive protocols, due to the high number of small local energy producers (e.g., solar panels on house roofs) that now interact with the classic large power-plants.
- Disaster relief operations, where data collected by sensor networks can be used to guide the actions of human operators and/or to operate automated rescue equipment.
- Surveillance using swarms of Unmanned Aerial Vehicles (UAVs), where sensor information (from sensors on the ground and/or on-board) can be used to guide the UAVs to accomplish their mission.
- Environmental monitoring and exploration using self-organized fleets of Autonomous Underwater Vehicles (AUVs), collaborating in order to reach a goal such as finding a pollutant source or tracing a seabed map.
- Infrastructure security and protection using smart camera networks, where the images collected are shared among the cameras and used to control the cameras themselves (pan-tilt-zoom) and ensure tracking of potential threats.

In particular, NECS team is currently focusing in the areas described in detail below.

4.2. Intelligent transportation systems

Throughout the world, roadways are notorious for their congestion, from dense urban network to large freeway systems. This situation tends to get worse over time due to the continuous increase of transportation demand whereas public investments are decreasing and space is lacking to build new infrastructures. The most obvious impact of traffic congestion for citizens is the increase of travel times and fuel consumption. Another critical effect is that infrastructures are not operated at their capacity during congestion, implying that fewer vehicles are served than the amount they were designed for. Using macroscopic fluid-like models, the NECS team has initiated new researches to develop innovative traffic management policies able to improve the infrastructure operations. The research activity is on two main challenges: (1) modeling and forecasting, so as to provide accurate information to users, e.g., travel times; and (2) control, via ramp-metering and/or variable speed limits. The Grenoble Traffic Lab (see http://necs.inrialpes.fr/pages/grenoble-traffic-lab.php) is an experimental platform, collecting traffic infrastructure information in real time from Grenoble South Ring, together with innovative software e.g. for travel-time prediciton, and a show-case where to graphically illustrate results to the end-user. This activity is done in close collaboration with local traffic authorities (DIR-CE, CG38, La Metro), and with the start-up company Karrus (http://www.karrus-its.com/)

4.3. Inertial navigation

The team is exploring techniques and approaches from estimation, filtering and machine learning, in order to use inertial sensor units in pedestrian navigation, attitude estimation, augmented reality and human activities recognition. These units are composed of accelerometers, magnetometers and gyroscopes, sensors that we find usually in smartphones. This area of research in the team will evolve towards multimodal navigation, cooperative and collaborative navigation in indoor and outdoor environments.

NON-A POST Team (section vide)

QUANTIC Project-Team

4. Application Domains

4.1. Quantum engineering

A new field of quantum systems engineering has emerged during the last few decades. This field englobes a wide range of applications including nano-electromechanical devices, nuclear magnetic resonance applications, quantum chemical synthesis, high resolution measurement devices and finally quantum information processing devices for implementing quantum computation and quantum communication. Recent theoretical and experimental achievements have shown that the quantum dynamics can be studied within the framework of estimation and control theory, but give rise to new models that have not been fully explored yet.

The QUANTIC team's activities are defined at the border between theoretical and experimental efforts of this emerging field with an emphasis on the applications in quantum information, computation and communication. The main objective of this interdisciplinary team is to develop quantum devices ensuring a robust processing of quantum information.

On the theory side, this is done by following a system theory approach: we develop estimation and control tools adapted to particular features of quantum systems. The most important features, requiring the development of new engineering methods, are related to the concept of measurement and feedback for composite quantum systems. The destructive and partial [0] nature of measurements for quantum systems lead to major difficulties in extending classical control theory tools. Indeed, design of appropriate measurement protocols and, in the sequel, the corresponding quantum filters estimating the state of the system from the partial measurement record, are themselves building blocks of the quantum system theory to be developed.

On the experimental side, we develop new quantum information processing devices based on quantum superconducting circuits. Indeed, by realizing superconducting circuits at low temperatures and using microwave measurement techniques, the macroscopic and collective degrees of freedom such as the voltage and the current are forced to behave according to the laws of quantum mechanics. Our quantum devices are aimed to protect and process quantum information through these integrated circuits.

[0] Here the partiality means that no single quantum measurement is capable of providing the complete information on the state of the system.

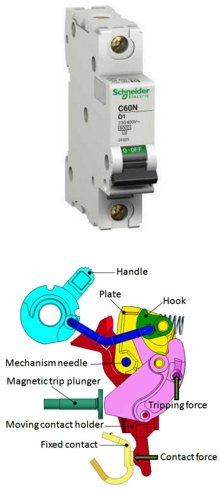
SPHINX Project-Team (section vide)

TRIPOP Team

4. Application Domains

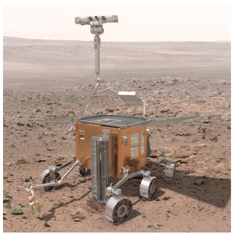
4.1. Applications Domains

Nonsmooth dynamical systems arise in a lot of application fields. *We briefly expose here some applications that have been treated in the BIPOP team and that we will continue in the TRIPOP team, as a validation for the research axes and also in terms of transfer (Sect. 7.1).* In mechanics, the main instances of nonsmooth dynamical systems are multibody systems with Signorini's unilateral contact, set-valued (Coulomb-like) friction and impacts, or in continuum mechanics, ideal plasticity, fracture or damage. Some illustrations are given in Figure 4 (a-f). Other instances of nonsmooth dynamical systems can also be found in electrical circuits with ideal components (see Figure 4 (g)) and in control theory, mainly with sliding mode control and variable structure systems (see Figure 4 (h)). More generally, every time a piecewise, possibly set–valued, model of systems is invoked, we end up with a nonsmooth system. This is the case, for instance, for hybrid systems in nonlinear control or for piecewise linear modeling of gene regulatory networks in mathematical biology (see Figure 4 (i)). Another common example of nonsmooth dynamics is also found when the vector field of a dynamical system is defined as a solution of an optimization problem under constraints, or a variational inequality. Examples of this kind are found in the optimal control theory, in dynamic Nash equilibrium or in the theory of dynamic flows over networks.

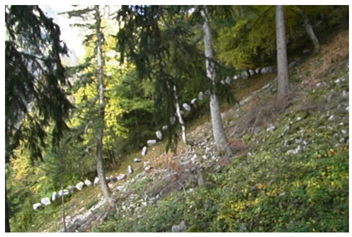


(a) Circuit breakers mechanisms [40]

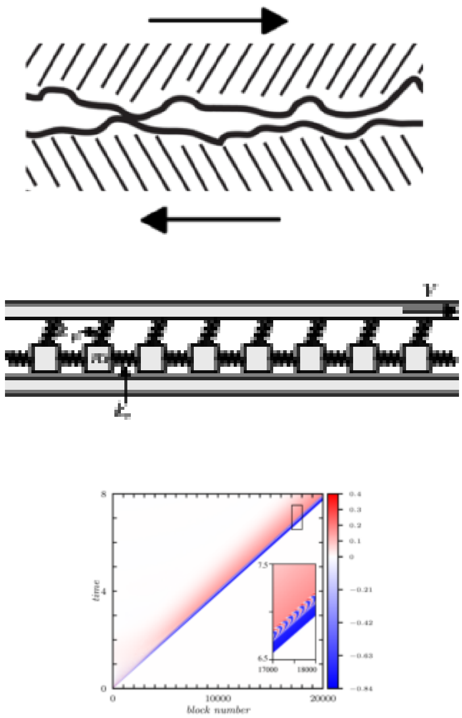
(b) Granular flows



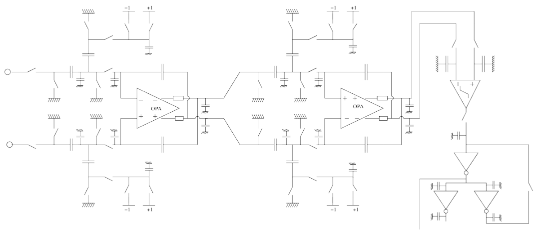
(c) Robots (ESA ExoMars Rover [35])



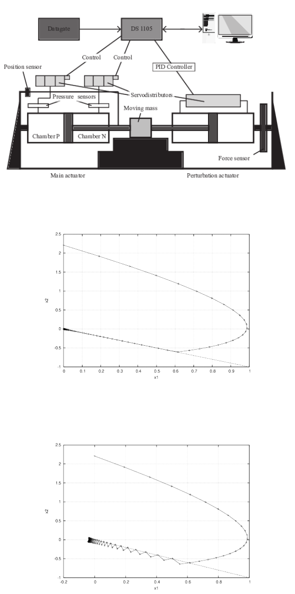
(d) Rockfall [47], [46], [59]



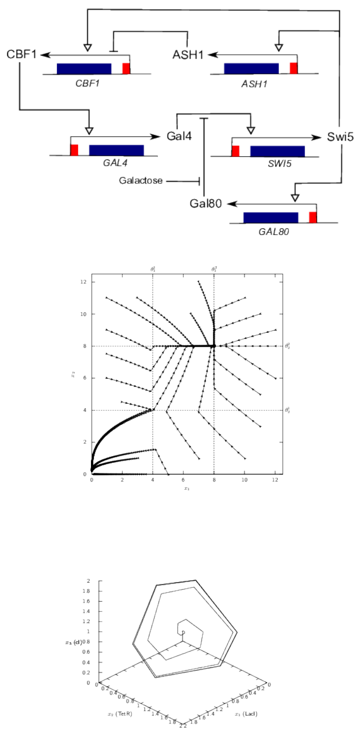
(e) Frictional interface and solitary waves in the Burridge-Knopoff model [81]



(a) Switched electrical circuits (delta-sigma converter) [29]



(b) Sliding mode control [32], [34], [70], [71], [80]



TROPICAL Project-Team

4. Application Domains

4.1. Discrete event systems (manufacturing systems, networks)

One important class of applications of max-plus algebra comes from discrete event dynamical systems [62]. In particular, modelling timed systems subject to synchronization and concurrency phenomena leads to studying dynamical systems that are non-smooth, but which have remarkable structural properties (nonexpansiveness in certain metrics , monotonicity) or combinatorial properties. Algebraic methods allow one to obtain analytical expressions for performance measures (throughput, waiting time, etc). A recent application, to emergency call centers, can be found in [55].

4.2. Optimal control and games

Optimal control and game theory have numerous well established applications fields: mathematical economy and finance, stock optimization, optimization of networks, decision making, etc. In most of these applications, one needs either to derive analytical or qualitative properties of solutions, or design exact or approximation algorithms adapted to large scale problems.

4.3. Operations Research

We develop, or have developed, several aspects of operations research, including the application of stochastic control to optimal pricing, optimal measurement in networks [122]. Applications of tropical methods arise in particular from discrete optimization [68], [69], scheduling problems with and-or constraints [114], or product mix auctions [130].

4.4. Computing program and dynamical systems invariants

A number of programs and systems verification questions, in which safety considerations are involved, reduce to computing invariant subsets of dynamical systems. This approach appears in various guises in computer science, for instance in static analysis of program by abstract interpretation, along the lines of P. and R. Cousot [75], but also in control (eg, computing safety regions by solving Isaacs PDEs). These invariant sets are often sought in some tractable effective class: ellipsoids, polyhedra, parametric classes of polyhedra with a controlled complexity (the so called "templates" introduced by Sankaranarayanan, Sipma and Manna [123]), shadows of sets represented by linear matrix inequalities, disjunctive constraints represented by tropical polyhedra [57], etc. The computation of invariants boils down to solving large scale fixed point problems. The latter are of the same nature as the ones encountered in the theory of zero-sum games, and so, the techniques developed in the previous research directions (especially methods of monotonicity, nonexpansiveness, discretization of PDEs, etc) apply to the present setting, see e.g. [90], [95] for the application of policy iteration type algorithms, or for the application for fixed point problems over the space of quadratic forms [7]. The problem of computation of invariants is indeed a key issue needing the methods of several fields: convex and nonconvex programming, semidefinite programming and symbolic computation (to handle semialgebraic invariants), nonlinear fixed point theory, approximation theory, tropical methods (to handle disjunctions), and formal proof (to certify numerical invariants or inequalities).

BONUS Team

4. Application Domains

4.1. Introduction

For the validation of our findings we obviously use standard benchmarks to facilitate the comparison with related works. In addition, we also target real-world applications in the context of our collaborations and industrial contracts. From the *application* point of view two classes are targeted: *complex scheduling* and *engineering design*. The objective is twofold: proposing new models for complex problems and solving efficiently BOPs using jointly the three lines of our research program. In the following, are given some use cases that are the focus of our current industrial collaborations.

4.2. Big optimization for complex scheduling

Three application domains are targeted: energy, health and transport and logistics. In the **energy** field, with the smart grid revolution (multi-)house energy management is gaining a growing interest. The key challenge is to make elastic with respect to the energy market the (multi-)house energy consumption and management. *This kind of demand-side management will be of strategic importance for energy companies in the near future.* In collaboration with the EDF energy company we are working on the formulation and solving of optimization problems on demand-side management in smart micro-grids for single- and multi-user frameworks. These complex problems require taking into account multiple conflicting objectives and constraints and many (deterministic/uncertain, discrete/continuous) parameters. A representative example of such BOPs that we are addressing is the scheduling of the activation of a large number of electrical and thermal appliances for a set of homes optimizing at least three criteria: maximizing the user's confort, minimizing its energy bill and minimzing peak consumption situations. In the **health** care domain, we are collaborating with the Beckman & Coulter company on the design and planning of large medical laboratories. This is a hot topic resulting from the mutualisation phenomenon which makes bigger these laboratories. As a consequence, being responsible for analyzing medical tests ordered by physicians on patient's samples, these laboratories receive large amounts of prescriptions and tubes making their associated workflow more complex. Our aim is therefore to design and plan any medical laboratory to minimize the costs and time required to perform the tests. More exactly, the focus is put on the multi-objective modeling and solving of large (e.g. dozens of thousands of medical test tubes to be analyzed) strategic, tactical and operational problems such as the layout design, machine selection and confguration, assignment and scheduling. Finally, in **transport and logistics**, within the context of our potential collaboration (being set up) with the EXOTEC company we target the optimization of the robotic logistics of 3D warehouses. More exactly, the problem consists in efficient complex scheduling without collision of thousands of missions realized by a fleet of dozens of robots and several operators in a 3D logistics warehouse. The problem is identified in the literature as the parts-to-picker based order processing in a rack-moving mobile robots environment.

4.3. Big optimization for engineering design

The focus is for now put on the aerospace vehicle design, a complex multidisciplinary optimization process, we are exploring in collaboration with ONERA. The objective is to find the vehicle architecture and characteristics that provide the optimal performance (flight performance, safety, reliability, cost, etc.) while satisfying design requirements [39]. A representative topic we are investigating, and will continue to investigate throughout the lifetime of the project given its complexity, is the design of launch vehicles that involves at least 4 tightly coupled disciplines (aerodynamics, structure, propulsion and trajectory). Each discipline may rely on time-demanding simulations such as Finite Element analyses (structure) and Computational Fluid Dynamics analyses (aerodynamics). Surrogate-assisted optimization is highly required to reduce the time complexity. In addition, the problem is high-dimensional (dozens of parameters and more than 3 objectives) requiring different decomposition schema (coupling *vs.* local variables, continuous *vs.* discrete even categorial variables, scalarization of the objectives). Another major issue arising in this area is the non-stationarity of the objective functions which is generally due to the abrupt change of a physical property that often occurs in the design of launch vehicles. In the same spirit than deep learning using neural networks, we use Deep Gaussian Processes to deal with non-stationary multi-objective functions. Finally, the resolution of the problem using only one objective takes 1 week using a multi-core processor. Therefore, *in addition to surrogates ultra-scale computing is required at different levels to speed up the search and improve the reliability which is a major requirement in aerospace design.* This example shows that we need to use the synergy between the 3 lines of our research program to tackle such BOPs.

GEOSTAT Project-Team

4. Application Domains

4.1. Sparse signals & optimisation

This research topic involves **Geostat** team and is used to set up an InnovationLab with I2S company

Sparsity can be used in many ways and there exist various sparse models in the literature; for instance minimizing the l_0 quasi-norm is known to be an NP-hard problem as one needs to try all the possible combinations of the signal's elements. The l_1 norm, which is the convex relation of the l_0 quasi-norm results in a tractable optimization problem. The l_p pseudo-norms with $0 < p < 1$ are particularly interesting as they give closer approximation of l_0 but result in a non-convex minimization problem. Thus, finding a global minimum for this kind of problem is not guaranteed. However, using a non-convex penalty instead of the l_1 norm has been shown to improve significantly various sparsity-based applications. Nonconvexity has a lot of statistical implications in signal and image processing. Indeed, natural images tend to have a heavy-tailed (kurtotic) distribution in certain domains such as wavelets and gradients. Using the l_1 norm comes to consider a Laplacian distribution. More generally, the hyper-Laplacian distribution is related to the l_p pseudo-norm ($0 < p < 1$) where the value of p controls how the distribution is heavy-tailed. As the hyper-Laplacian distribution for $0 < p < 1$ represents better the empirical distribution of the transformed images, it makes sense to use the l_p pseudo-norms instead of l_1. Other functions that better reflect heavy-tailed distributions of images have been used as well such as Student-t or Gaussian Scale Mixtures. The internal properties of natural images have helped researchers to push the sparsity principle further and develop highly efficient algorithms for restoration, representation and coding. Group sparsity is an extension of the sparsity principle where data is clustered into groups and each group is sparsified differently. More specifically, in many cases, it makes sense to follow a certain structure when sparsifying by forcing similar sets of points to be zeros or non-zeros simultaneously. This is typically true for natural images that represent coherent structures. The concept of group sparsity has been first used for simultaneously shrinking groups of wavelet coefficients because of the relations between wavelet basis elements. Lastly, there is a strong relationship between sparsity, nonpredictability and scale invariance.

We have shown that the two powerful concepts of sparsity and scale invariance can be exploited to design fast and efficient imaging algorithms. A general framework has been set up for using non-convex sparsity by applying a first-order approximation. When using a proximal solver to estimate a solution of a sparsity-based optimization problem, sparse terms are always separated in subproblems that take the form of a proximal operator. Estimating the proximal operator associated to a non-convex term is thus the key component to use efficient solvers for non-convex sparse optimization. Using this strategy, only the shrinkage operator changes and thus the solver has the same complexity for both the convex and non-convex cases. While few previous works have also proposed to use non-convex sparsity, their choice of the sparse penalty is rather limited to functions like the l_p pseudo-norm for certain values of $p \geq 0.5$ or the Minimax Concave (MC) penalty because they admit an analytical solution. Using a first-order approximation only requires calculating the (super)gradient of the function, which makes it possible to use a wide range of penalties for sparse regularization. This is important in various applications where we need a flexible shrinkage function such as in edge-aware processing. Apart from non-convexity, using a first-order approximation makes it easier to verify the optimality condition of proximal operator-based solvers via fixed-point interpretation. Another problem that arises in various imaging applications but has attracted less works is the problem of multi-sparsity, when the minimization problem includes various sparse terms that can be non-convex. This is typically the case when looking for a sparse solution in a certain domain while rejecting outliers in the data-fitting term. By using one intermediate variable per sparse term, we show that proximal-based solvers can be efficient. We give a detailed study of the Alternating Direction Method of Multipliers (ADMM) solver for multi-sparsity and study its properties. The following subjects are addressed and receive new solutions:

- **Edge aware smoothing**: given an input image g, one seeks a smooth image u "close" to g by minimizing:

$$\underset{u}{\text{argmin}}\ \frac{\lambda}{2}\|u-g\|_2^2+\psi(\nabla u)$$

where ψ is a sparcity-inducing non-convex function and λ a positive parameter. Splitting and alternate minimization lead to the sub-problems:

$$\begin{aligned}
(\text{sp1}) &\quad : \quad v^{(k+1)} \longleftarrow \underset{v}{\text{argmin}}\ \psi(v)+\frac{\beta}{2}\|\nabla u^{(k)}-v\|_2^2 \\
(\text{sp2}) &\quad : \quad u^{(k+1)} \longleftarrow \underset{u}{\text{argmin}}\ \lambda\|u-g\|_2^2+\beta\|\nabla u-v^{(k+1)}\|_2^2.
\end{aligned}$$

We solve sub-problem (sp2) through deconvolution and efficient estimation via separable filters and warm-start initialization for fast GPU implementation, and sub-problem (sp1) through non-convex proximal form.

- **Structure-texture separation**: gesign of an efficient algorithm using non-convex terms on both the data-fitting and the prior. The resulting problem is solved via a combination of Half-Quadratic (HQ) and Maximization-Minimization (MM) methods. We extract challenging texture layers outperforming existing techniques while maintaining a low computational cost. Using spectral sparsity in the framework of low-rank estimation, we propose to use robust Principal Component Analysis (RPCA) to perform robust separation on multi-channel images such as glare and artifacts removal of flash/no-flash photographs. As in this case, the matrix to decompose has much less columns than lines, we propose to use a QR decomposition trick instead of a direct singular value decomposition (SVD) which makes the decomposition faster.

- **Robust integration**: in many applications, we need to reconstruct an image from corrupted gradient fields. The corruption can take the form of outliers only when the vector field is the result of transformed gradient fields (low-level vision), or mixed outliers and noise when the field is estimated from corrupted measurements (surface reconstruction, gradient camera, Magnetic Resonance Imaging (MRI) compressed sensing, etc.). We use non-convexity and multi-sparsity to build efficient integrability enforcement algorithms. We present two algorithms : 1) a local algorithm that uses sparsity in the gradient field as a prior together with a sparse data-fitting term, 2) a non-local algorithm that uses sparsity in the spectral domain of non-local patches as a prior together with a sparse data-fitting term. Both methods make use of a multi-sparse version of the Half-Quadratic solver. The proposed methods were the first in the literature to propose a sparse regularization to improve integration. Results produced with these methods significantly outperform previous works that use no regularization or simple l_1 minimization. Exact or near-exact recovery of surfaces is possible with the proposed methods from highly corrupted gradient fields with outliers.

- **Learning image denoising**: deep convolutional networks that consist in extracting features by repeated convolutions with high-pass filters and pooling/downsampling operators have shown to give near-human recognition rates. Training the filters of a multi-layer network is costly and requires powerful machines. However, visualizing the first layers of the filters shows that they resemble wavelet filters, leading to sparse representations in each layer. We propose to use the concept of scale invariance of multifractals to extract invariant features on each sparse representation. We build a bi-Lipschitz invariant descriptor based on the distribution of the singularities of the sparsified images in each layer. Combining the descriptors of each layer in one feature vector leads to a compact representation of a texture image that is invariant to various transformations. Using this descriptor that is efficient to calculate with learning techniques such as classifiers combination and artificially adding training data, we build a powerful texture recognition system that outperforms previous works on 3 challenging datasets. In fact, this system leads to quite close recognition rates compared to latest advanced deep nets while not requiring any filters training.

INOCS Project-Team

4. Application Domains

4.1. Energy

In energy, the team mainly focuses on pricing models for demand side management. Demand side management methods are traditionally used to control electricity demand which became quite irregular recently and resulted in inefficiency in supply. We have explored the relationship between energy suppliers and customers who are connected to a smart grid. The smart grid technology allows customers to keep track of hourly prices and shift their demand accordingly, and allows the provider to observe the actual demand response to its pricing strategy. We tackle pricing problems in energy according to the bilevel optimization approaches. Some research works in this domain are supported by bilateral grants with EDF.

4.2. Transportation and Logistics

In transportation and logistics, the team addresses mainly integrated problems, which require taking into account simultaneously different types of decision. Examples are location and routing, inventory management and routing or staff scheduling and warehouse operations management. Such problems occur from the supply chain design level to the logistic facility level. Some research activities in this application domain are supported by bilateral grants/contracts with Colisweb, DHL, HappyChic, INFRABEL, and Kéolis.

4.3. Telecommunications

In telecommunications, the team mainly focuses on network design problems and on routing problems. Such problems are optimization problems with complex structure, since the optimization of capacity installation and traffic flow routing have to be addressed simultaneously. Some research works are conducted within a long-term cooperation with Nokia (formerly Alcatel-Lucent Bell Labs).

MISTIS Project-Team

4. Application Domains

4.1. Image Analysis

Participants: Alexis Arnaud, Veronica Munoz Ramirez, Florence Forbes, Stéphane Girard, Jaime Eduardo Arias Almeida, Pierre-Antoine Rodesch, Hongliang Lu, Fabien Boux, Benoit Kugler, Alexandre Constantin.

As regards applications, several areas of image analysis can be covered using the tools developed in the team. More specifically, in collaboration with team PERCEPTION, we address various issues in computer vision involving Bayesian modelling and probabilistic clustering techniques. Other applications in medical imaging are natural. We work more specifically on MRI and functional MRI data, in collaboration with the Grenoble Institute of Neuroscience (GIN) and the NeuroSpin center of CEA Saclay. We also consider other statistical 2D fields coming from other domains such as remote sensing, in collaboration with the Institut de Planétologie et d'Astrophysique de Grenoble (IPAG) and the Centre National d'Etudes Spatiales (CNES). In this context, we worked on hyperspectral and/or multitemporal images. In the context of the "pole de competivité" project I-VP, we worked of images of PC Boards. We also address reconstruction problems in tomography with CEA Grenoble.

4.2. Multi sensor Data Analysis

Participants: Jean-Michel Bécu, Florence Forbes, Thibaud Rahier, Hongliang Lu, Fatima Fofana.

A number of our methods are at the the intersection of data fusion, statistics, machine learning and acoustic signal processing. The context can be the surveillance and monitoring of a zone acoustic state from data acquired at a continuous rate by a set of sensors that are potentially mobile and of different nature (eg WIFUZ project with the ACOEM company in the context of a DGA-rapid initiative). Typical objectives include the development of prototypes for surveillance and monitoring that are able to combine multi sensor data coming from acoustic sensors (microphones and antennas) and optical sensors (infrared cameras) and to distribute the processing to multiple algorithmic blocs. Our interest in acoustic data analysis mainly started from past European projects, POP and Humavips, in collaboration with the PERCEPTION team (PhD theses of Vassil Khalidov, Ramya Narasimha, Antoine Deleforge, Xavier Alameda, and Israel Gebru).

4.3. Biology, Environment and Medicine

Participants: Jaime Eduardo Arias Almeida, Alexis Arnaud, Florence Forbes, Stéphane Girard, Jean-Baptiste Durand, Clément Albert, Julyan Arbel, Jean-Michel Bécu, Thibaud Rahier, Brice Olivier, Karina Ashurbekova, Fabien Boux, Veronica Munoz Ramirez, Fei Zheng.

A third domain of applications concerns biology and medicine. We considered the use of mixture models to identify biomakers. We also investigated statistical tools for the analysis of fluorescence signals in molecular biology. Applications in neurosciences are also considered. In the environmental domain, we considered the modelling of high-impact weather events and the use of hyperspectral data as a new tool for quantitative ecology.

MODAL Project-Team

4. Application Domains

4.1. Economic World

The Modal team applies it research to the economic world through CIFRE Phd supervision such as CACF (credit scoring), A-Volute (expert in 3D sound), Meilleur Taux (insurance comparator), ...It also has many contracts with companies such as Decathlon (world leader in sports equipment), Arcelor-Mittal (steel industry) or Alstom (integrated transport systems).

4.2. Biology

The second main application domain of the team is the biology. Members of the team are involved in the supervision and scientific animation of the bilille platform, the bioinformatics and bioanalysis platform of Lille.

RANDOPT Team

4. Application Domains

4.1. Application Domains

Applications of black-box algorithms occur in various domains. Industry but also researchers in other academic domains have therefore a great need to apply black-box algorithms on a daily basis. We see this as a great source of motivation to design better methods. Applications not only allow us to backup our methods and understand what are the relevant features to solve a real-world problem but also help identify novel difficulties or set priorities in terms of algorithm design.

Asides from the two applications to Machine Learning that we detail below, we however do not target a specific application domain and we are interested in possible black-box applications stemming from various origins. This is for us intrinsic to the nature of the methods we develop that are general purpose algorithms. Hence our strategy with respect to applications can be seen as opportunistic and our main selection criteria when approached by colleagues who want to develop a collaboration around an application is whether we judge the application interesting: that is the application brings new challenges and/or gives us the opportunity to work on topics we already intended to work on.

The three concrete applications related to industrial collaborations we are currently dealing with are:

- With EDF R&D through the design and placement of bi-facial photovoltaic panel for the postdoc of Asma Atamna funded by the PGMO project.
- With Thales for the thesis of Konstantinos Varelas (DGA-CIFRE thesis) related to the design of radars (shape optimization of the wave form). This thesis investigates the development of large-scale variants of CMA-ES.
- With Storengy, a subsidiary of Engie specialized in gas storage for the thesis of Cheikh Touré. Different multi-objective applications are considered in this context but the primary motivation of Storengy is to get at their disposal a better multi-objective variant of CMA-ES which is the main objective of the developments within the thesis.

Additionally, there are two specific types of applications stemming from Machine Learning we would like to focus on: problems with non-differentiable loss that can occur in reinforcement learning and hyperparameter tuning problems. For the first class of problems the motivation comes from the paper [36] where different reinforcement learning problems are addressed and the weights of neural networks are adjusted using evolution strategies. Those problems are large-scale (in [36] up to 10^6 weights are adjusted), and the large-scale variants of CMA-ES we want to investigate might be relevant in this case. For the second class of problems (hyperparameter tuning problems), standard approches to handle those problems are Bayesian optimization algorithms but despite the tremendous effort for developing Bayesian optimization techniques and having implementations of Bayesian optimization algorithms within libraries, pure random search is still often used for training neural networks. One reason is that pure random search is intrinsically parallel [18]. This suggests that methods like CMA-ES—that are also intrinsically parallel—can be also advantageously used for hyperparameter tuning: this was demonstrated to tune deep neural networks in [32]. One limitation though of the CMA-ES algorithm is that it cannot deal with categorical/integer and continuous variables at the same time. This motivates us to investigate the development of CMA-ES variants that are able to deal with mixed variables.

When dealing with single applications, the results observed are difficult to generalize: typically not many methods are tested on a single application as tests are often time consuming and performed in restrictive settings. Yet, if one circumvent the problem of confidentiality of data and of criticality for companies to publish their applications, real-world problems could become benchmarks as any other analytical function. This would allow to test wider ranges of methods on the problems and to find out whether analytical benchmarks properly capture real-world problem difficulties. We will thus seek to incorporate real-world problems within the COCO platform. This is a recurrent demand by researchers in optimization. As far as confidentiality of data are concerned, our preliminary discussions with industrials allow us to be optimistic that we can convince industrials to propose real-world problems with anonymized (and uncritical) data that still capture the essence of the underlying real-world problem.

REALOPT Project-Team

4. Application Domains

4.1. Network Design and Routing Problems

We are actively working on problems arising in network topology design, implementing a survivability condition of the form “at least two paths link each pair of terminals”. We have extended polyhedral approaches to problem variants with bounded length requirements and re-routing restrictions [46]. Associated to network design is the question of traffic routing in the network: one needs to check that the network capacity suffices to carry the demand for traffic. The assignment of traffic also implies the installation of specific hardware at transient or terminal nodes.

To accommodate the increase of traffic in telecommunication networks, today’s optical networks use grooming and wavelength division multiplexing technologies. Packing multiple requests together in the same optical stream requires to convert the signal in the electrical domain at each aggregation of disaggregation of traffic at an origin, a destination or a bifurcation node. Traffic grooming and routing decisions along with wavelength assignments must be optimized to reduce opto-electronics system installation cost. We developed and compared several decomposition approaches [73], [71], [70] to deal with backbone optical network with relatively few nodes (around 20) but thousands of requests for which traditional multi-commodity network flow approaches are completely overwhelmed. We also studied the impact of imposing a restriction on the number of optical hops in any request route [69]. We also developed a branch-and-cut approach to a problem that consists in placing sensors on the links of a network for a minimum cost [51], [52].

The Dial-a-Ride Problem is a variant of the pickup and delivery problem with time windows, where the user inconvenience must be taken into account. In [62], ride time and customer waiting time are modeled through both constraints and an associated penalty in the objective function. We develop a column generation approach, dynamically generating feasible vehicle routes. Handling ride time constraints explicitly in the pricing problem solver requires specific developments. Our dynamic programming approach for pricing problem makes use of a heuristic dominance rule and a heuristic enumeration procedure, which in turns implies that our overall branch-and-price procedure is a heuristic. However, in practice our heuristic solutions are experimentally very close to exact solutions and our approach is numerically competitive in terms of computation times.

In [60], [59], we consider the problem of covering an urban area with sectors under additional constraints. We adapt the aggregation method to our column generation algorithm and focus on the problem of disaggregating the dual solution returned by the aggregated master problem.

We studied several time dependent formulations for the unit demand vehicle routing problem [36], [35]. We gave new bounding flow inequalities for a single commodity flow formulation of the problem. We described their impact by projecting them on some other sets of variables, such as variables issued of the Picard and Queyranne formulation or the natural set of design variables. Some inequalities obtained by projection are facet defining for the polytope associated with the problem. We are now running more numerical experiments in order to validate in practice the efficiency of our theoretical results.

We also worked on the p-median problem, applying the matching theory to develop an efficient algorithm in Y-free graphs and to provide a simple polyhedral characterization of the problem and therefore a simple linear formulation [68] simplifying results from Baiou and Barahona.

We considered the multi-commodity transportation problem. Applications of this problem arise in, for example, rail freight service design, "less than truckload" trucking, where goods should be delivered between different locations in a transportation network using various kinds of vehicles of large capacity. A particularity here is that, to be profitable, transportation of goods should be consolidated. This means that goods are not delivered directly from the origin to the destination, but transferred from one vehicle to another in intermediate locations. We proposed an original Mixed Integer Programming formulation for this problem which is suitable for resolution by a Branch-and-Price algorithm and intelligent primal heuristics based on it.

For the problem of routing freight railcars, we proposed two algorithmes based on the column generation approach. These algorithmes have been tested on a set of real-life instances coming from a real Russian freight transportation company. Our algorithms have been faster on these instances than the current solution approach being used by the company.

4.2. Packing and Covering Problems

Realopt team has a strong experience on exact methods for cutting and packing problems. These problems occur in logistics (loading trucks), industry (wood or steel cutting), computer science (parallel processor scheduling).

We developed a branch-and-price algorithm for the Bin Packing Problem with Conflicts which improves on other approaches available in the literature [67]. The algorithm uses our methodological advances like the generic branching rule for the branch-and-price and the column based heuristic. One of the ingredients which contributes to the success of our method are fast algorithms we developed for solving the subproblem which is the Knapsack Problem with Conflicts. Two variants of the subproblem have been considered: with interval and arbitrary conflict graphs.

We also developed a branch-and-price algorithm for a variant of the bin-packing problem where the items are fragile. In [24] we studied empirically different branching schemes and different algorithms for solving the subproblems.

We studied a variant of the knapsack problem encountered in inventory routing problem [54]: we faced a multiple-class integer knapsack problem with setups [53] (items are partitioned into classes whose use implies a setup cost and associated capacity consumption). We showed the extent to which classical results for the knapsack problem can be generalized to this variant with setups and we developed a specialized branch-and-bound algorithm.

We studied the orthogonal knapsack problem, with the help of graph theory [48], [47], [50], [49]. Fekete and Schepers proposed to model multi-dimensional orthogonal placement problems by using an efficient representation of all geometrically symmetric solutions by a so called *packing class* involving one *interval graph* for each dimension. Though Fekete & Schepers' framework is very efficient, we have however identified several weaknesses in their algorithms: the most obvious one is that they do not take advantage of the different possibilities to represent interval graphs. We propose to represent these graphs by matrices with consecutive ones on each row. We proposed a branch-and-bound algorithm for the 2D knapsack problem that uses our 2D packing feasibility check. We are currently developing exact optimization tools for glass-cutting problems in a collaboration with Saint-Gobain [29]. This 2D-3stage-Guillotine cut problems are very hard to solve given the scale of the instance we have to deal with. Moreover one has to issue cutting patterns that avoid the defaults that are present in the glass sheet that are used as raw material. There are extra sequencing constraints regarding the production that make the problem even more complex.
We have also organized a European challenge on packing with society Renault: see https://paginas.fe.up.pt/~esicup/extern/esicup-12thMeeting/pmwiki.php?n=Conference.Info. This challenge is about loading trucks under practical constraints.

4.3. Planning, Scheduling, and Logistic Problems

Inventory routing problems combine the optimization of product deliveries (or pickups) with inventory control at customer sites. We considered an industrial application where one must construct the planning of single product pickups over time; each site accumulates stock at a deterministic rate; the stock is emptied on each visit. We have developed a branch-and-price algorithm where periodic plans are generated for vehicles by solving a multiple choice knapsack subproblem, and the global planning of customer visits is coordinated by the master program [55]. We previously developed approximate solutions to a related problem combining vehicle routing and planning over a fixed time horizon (solving instances involving up to 6000 pick-ups and deliveries to plan over a twenty day time horizon with specific requirements on the frequency of visits to customers [57].

Together with our partner company GAPSO from the associate team SAMBA, we worked on the equipment routing task scheduling problem [61] arising during port operations. In this problem, a set of tasks needs to be performed using equipments of different types with the objective to maximize the weighted sum of performed tasks.

We participated to the project on an airborne radar scheduling. For this problem, we developed fast heuristics [45] and exact algorithms [26]. A substantial research has been done on machine scheduling problems. A new compact MIP formulation was proposed for a large class of these problems [25]. An exact decomposition algorithm was developed for the NP-hard maximizing the weighted number of late jobs problem on a single machine [63]. A dominant class of schedules for malleable parallel jobs was discovered in the NP-hard problem to minimize the total weighted completion time [65]. We proved that a special case of the scheduling problem at cross docking terminals to minimize the storage cost is polynomially solvable [66], [64].

Another application area in which we have successfully developed MIP approaches is in the area of tactical production and supply chain planning. In [23], we proposed a simple heuristic for challenging multi-echelon problems that makes effective use of a standard MIP solver. [22] contains a detailed investigation of what makes solving the MIP formulations of such problems challenging; it provides a survey of the known methods for strengthening formulations for these applications, and it also pinpoints the specific substructure that seems to cause the bottleneck in solving these models. Finally, the results of [30] provide demonstrably stronger formulations for some problem classes than any previously proposed. We are now working on planning phytosanitary treatments in vineries.

We have been developing robust optimization models and methods to deal with a number of applications like the above in which uncertainty is involved. In [41], [40], we analyzed fundamental MIP models that incorporate uncertainty and we have exploited the structure of the stochastic formulation of the problems in order to derive algorithms and strong formulations for these and related problems. These results appear to be the first of their kind for structured stochastic MIP models. In addition, we have engaged in successful research to apply concepts such as these to health care logistics [31]. We considered train timetabling problems and their re-optimization after a perturbation in the network [43], [42]. The question of formulation is central. Models of the literature are not satisfactory: continuous time formulations have poor quality due to the presence of discrete decision (re-sequencing or re-routing); arc flow in time-space graph blow-up in size (they can only handle a single line timetabling problem). We have developed a discrete time formulation that strikes a compromise between these two previous models. Based on various time and network aggregation strategies, we develop a 2-stage approach, solving the contiguous time model having fixed the precedence based on a solution to the discrete time model.

Currently, we are conducting investigations on a real-world planning problem in the domain of energy production, in the context of a collaboration with EDF [37], [38], [39]. The problem consists in scheduling maintenance periods of nuclear power plants as well as production levels of both nuclear and conventional power plants in order to meet a power demand, so as to minimize the total production cost. For this application, we used a Dantzig-Wolfe reformulation which allows us to solve realistic instances of the deterministic version of the problem [44]. In practice, the input data comprises a number of uncertain parameters. We deal with a scenario-based stochastic demand with help of a Benders decomposition method. We are working on Multistage Robust Optimization approaches to take into account other uncertain parameters like the duration of each maintenance period, in a dynamic optimization framework. The main challenge addressed in this work is the joint management of different reformulations and solving techniques coming from the deterministic (Dantzig-Wolfe decomposition, due to the large scale nature of the problem), stochastic (Benders decomposition, due to the number of demand scenarios) and robust (reformulations based on duality and/or column and/or row generation due to maintenance extension scenarios) components of the problem [32].

4.4. Resource Allocation for High Performance and Cloud Computing

In the context of numerical simulations on high performance machines, optimizing data locality and resource usage is very important for faster execution times and lower energy consumption. This optimization can be seen as a special case of scheduling problem on parallel resource, with several challenges. First, instances are typically large: a large matrix factorization (with 50×50 blocks) involves about $30 \cdot 10^3$ tasks. Then, HPC platforms consist of heterogeneous and unrelated resources, what is known to make scheduling problems hard to approximate. Finally, due to co-scheduling effects and shared communication resources, it is not realistic to accurately model the exact duration of tasks. All these observations make it impossible to rely on static optimal solutions, and HPC applications have gone from simple generic static allocations to runtime dynamic scheduling strategies that make their decisions based on the current state of the platform (the location of input data), the expected transfer and running times for the tasks, and some affinity and priority information that have possibly been computed offline. In this context, we are strongly involved in the design of scheduling strategies for the StarPU runtime, with two goals: proving that it is possible to design approximation algorithms whose complexity is extremely small (typically sub-linear in the number of ready tasks), and show that they can be used in practice with good performance results. We are pursuing collaborations both with teams developing the StarPU system (Storm) by designing algorithms for the generic scheduling problems [28], and with teams developing linear algebra algorithms over the runtime (Hiepacs), by proposing specialized algorithms for specific cases. For example, in the case of linear algebra applications on heterogeneous platforms, we have considered the combinatorial optimization problem associated to matrix multiplication, that is amenable to partitioning the unit square into zones of prescribed areas while minimizing the overall size of the boundaries. We have improved the best known approximation ratio to 1.15 in [27] and we have shown that the resulting distribution schemes can indeed be used to design efficient implementations using StarPU in [34].

SELECT Project-Team

4. Application Domains

4.1. Introduction

A key goal of SELECT is to produce methodological contributions in statistics. For this reason, the SELECT team works with applications that serve as an important source of interesting practical problems and require innovative methodology to address them. Many of our applications involve contracts with industrial partners, e.g., in reliability, although we also have several academic collaborations, e.g., in genetics and image analysis.

4.2. Curve classification

The field of classification for complex data such as curves, functions, spectra and time series, is an important problem in current research. Standard data analysis questions are being looked into anew, in order to define novel strategies that take the functional nature of such data into account. Functional data analysis addresses a variety of applied problems, including longitudinal studies, analysis of fMRI data, and spectral calibration.

We are focused in particular on unsupervised classification. In addition to standard questions such as the choice of the number of clusters, the norm for measuring the distance between two observations, and vectors for representing clusters, we must also address a major computational problem: the functional nature of the data, which requires new approaches.

4.3. Computer experiments and reliability

For several years now, SELECT has collaborated with the EDF-DER *Maintenance des Risques Industriels* group. One important theme involves the resolution of inverse problems using simulation tools to analyze incertainty in highly complex physical systems.

The other major theme concerns reliability, through a research collaboration with Nexter involving a Cifre convention. This collaboration concerns a lifetime analysis of a vehicle fleet to assess ageing.

Moreover, a collaboration is ongoing with Dassault Aviation on the modal analysis of mechanical structures, which aims to identify the vibration behavior of structures under dynamic excitation. From the algorithmic point of view, modal analysis amounts to estimation in parametric models on the basis of measured excitations and structural response data. In literature and existing implementations, the model selection problem associated with this estimation is currently treated by a rather weighty and heuristic procedure. In the context of our own research, model selection via penalization methods are being tested on this model selection problem.

4.4. Analysis of genomic data

For many years now, SELECT collaborates with Marie-Laure Martin-Magniette (URGV) for the analysis of genomic data. An important theme of this collaboration is using statistically sound model-based clustering methods to discover groups of co-expressed genes from microarray and high-throughput sequencing data. In particular, identifying biological entities that share similar profiles across several treatment conditions, such as co-expressed genes, may help identify groups of genes that are involved in the same biological processes.

SELECT collaborates with Anavaj Sakuntabhai and Philippe Dussart (Pasteur Institute) on predicting dengue severity using only low-dimensional clinical data obtained at hospital arrival. Further collaborations are underway in dengue fever and encephalitis with researchers at the Pasteur Institute, including with Jean-David Pommier.

SELECT is involved in the ANR “jeunes chercheurs” MixStatSeq directed by Cathy Maugis (INSA Toulouse), which is concerned with statistical analysis and clustering of RNASeq genomics data.

4.5. Pharmacovigilance

A collaboration is ongoing with Pascale Tubert-Bitter, Ismael Ahmed and Mohamed Sedki (Pharmacoepidemiology and Infectious Diseases, PhEMI) for the analysis of pharmacovigilance data. In this framework, the goal is to detect, as soon as possible, potential associations between certain drugs and adverse effects, which appeared after the authorized marketing of these drugs. Instead of working on aggregate data (contingency table) like is usually the case, the approach developed aims to deal with individual's data, which perhaps gives more information.

4.6. Spectroscopic imaging analysis of ancient materials

Ancient materials, encountered in archaeology and paleontology are often complex, heterogeneous and poorly characterized before physico-chemical analysis. A popular technique to gather as much physico-chemical information as possible, is spectro-microscopy or spectral imaging, where a full spectra, made of more than a thousand samples, is measured for each pixel. The produced data is tensorial with two or three spatial dimensions and one or more spectral dimensions, and requires the combination of an "image" approach with a "curve analysis" approach. Since 2010 SELECT, collaborates with Serge Cohen (IPANEMA) on clustering problems, taking spatial constraints into account.

SEQUEL Project-Team

4. Application Domains

4.1. Sequential decision making under uncertainty and prediction

The spectrum of applications of our research is very wide: it ranges from the core of our research, that is sequential decision making under uncertainty, to the application of components used to solve this decision making problem.

To be more specific, we work on computational advertising and recommendation systems; these problems are considered as a sequential matching problem in which resources available in a limited amount have to be matched to meet some users' expectations. The sequential approach we advocate paves the way to better tackle the cold-start problem, and non stationary environments. More generally, these approaches are applied to the optimization of budgeted resources under uncertainty, in a time-varying environment, including constraints on computational times (typically, a decision has to be made in less than 1 ms in a recommendation system). An other field of applications of our research is related to education which we consider as a sequential matching problem between a student, and educational contents.

The algorithms to solve these tasks heavily rely on tools from machine learning, statistics, and optimization. Henceforth, we also apply our work to more classical supervised learning, and prediction tasks, as well as unsupervised learning tasks. The whole range of methods is used, from decision forests, to kernel methods, to deep learning. For instance, we have recently used deep learning on images. We also have a line of works related to software development studying how machine learning can improve the quality of software being developed. More generally, we apply our research to data science.

SIERRA Project-Team

4. Application Domains

4.1. Applications for Machine Learning

Machine learning research can be conducted from two main perspectives: the first one, which has been dominant in the last 30 years, is to design learning algorithms and theories which are as generic as possible, the goal being to make as few assumptions as possible regarding the problems to be solved and to let data speak for themselves. This has led to many interesting methodological developments and successful applications. However, we believe that this strategy has reached its limit for many application domains, such as computer vision, bioinformatics, neuro-imaging, text and audio processing, which leads to the second perspective our team is built on: Research in machine learning theory and algorithms should be driven by interdisciplinary collaborations, so that specific prior knowledge may be properly introduced into the learning process, in particular with the following fields:

- Computer vision: object recognition, object detection, image segmentation, image/video processing, computational photography. In collaboration with the Willow project-team.
- Bioinformatics: cancer diagnosis, protein function prediction, virtual screening. In collaboration with Institut Curie.
- Text processing: document collection modeling, language models.
- Audio processing: source separation, speech/music processing.
- Neuro-imaging: brain-computer interface (fMRI, EEG, MEG).

TAU Team

4. Application Domains

4.1. Computational Social Sciences

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag, Paola Tubaro
Collaboration: Jean-Pierre Nadal (EHESS); Marco Cuturi, Bruno Crépon (ENSAE); Thierry Weil (Mines); Jean-Luc Bazet (RITM)

Computational Social Sciences (CSS) studies social and economic phenomena, ranging from technological innovation to politics, from media to social networks, from human resources to education, from inequalities to health. It combines perspectives from different scientific disciplines, building upon the tradition of computer simulation and modeling of complex social systems [99] on the one hand, and data science on the other hand, fueled by the capacity to collect and analyze massive amounts of digital data.

The emerging field of CSS raises formidable challenges along three dimensions. Firstly, the definition of the research questions, the formulation of hypotheses and the validation of the results require a tight pluridisciplinary interaction and dialogue between researchers from different backgrounds. Secondly, the development of CSS is a touchstone for ethical AI. On the one hand, CSS gains ground in major, data-rich private companies; on the other hand, public researchers around the world are engaging in an effort to use it for the benefit of society as a whole [119]. The key technical difficulties related to data and model biases, and to self-fulfilling prophecies have been discussed in section 3.1 . Thirdly, CSS does not only regard scientists: it is essential that the civil society participate in the science of society [146].

TAO was involved in CSS for the last five years, and its activities have been strengthened thanks to P. Tubaro's and I. Guyon's expertises respectively in sociology and economics, and in causal modeling. Details are given in Section 7.3 .

4.2. Energy Management

Participants: Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhD: Victor Berger, Benjamin Donnot, Balthazar Donon, Herilalaina Rakotoarison
Collaboration: Antoine Marot, Patrick Panciatici (RTE), Vincent Renault (Artelys), Olivier Teytaud (Facebook)

Energy Management has been an application domain of choice for TAO since the end 2000s, with main partners SME Artelys (METIS Ilab Inria; ADEME project POST; ADEME project NEXT) and RTE (See.4C European challenge; two CIFRE PhDs). The goals concern i) optimal planning over several spatio-temporal scales, from investments on continental Europe/North Africa grid at the decade scale (POST), to daily planning of local or regional power networks (NEXT); ii) monitoring and control of the French grid enforcing the prevention of power breaks (RTE); iii) improvement of house-made numerical methods using data-intense learning (as described in Section 3.2) in all aspects of IFPEN activities, from geological problems in oil prospection (IFPEN) to the optimal placement of eolians in eolian fields (IFPEN).
Optimal planning over long periods of time amounts to optimal sequential decision under high uncertainties, ranging from stochastic uncertainties (weather, market prices, demand prediction) handled based on massive data, to non-stochastic uncertainties (e.g., political decisions about the nuclear policy) handled through defining and selecting a tractable number of scenarios. Note that non-anticipativity constraints forbid the use of dynamic programming-related methods; this led to propose the *Direct Value Search* method [79] at the end of the POST project. A further recent work in the same direction [21] proposes and theoretically studies the *Direct Model Predictive Control* approach, a hybrid model which merges the properties of two different dynamic optimization methods, Model Predictive Control and Stochastic Dual Dynamic Programming, has robust convergence properties, and experimentally competes with both methods alone.

The daily maintainance of power grids requires the building of approximate predictive models on the top of any given network topology. Deep Networks are natural candidates for such modelling, considering the size of the French grid ($\sim$ 10000 nodes), but the representation of the topology is a challenge when, e.g. the RTE goal is to quickly ensure the "n-1" security constraint (the network should remain safe even if any of the 10000 nodes fails). Existing simulators are too slow to be used in real time, and the size of actual grids makes it intractable to train surrogate models for all possible (n-1) topologies (see Section 7.4 for more details).

Even when efficient simulators do exist, they need to be calibrated (adjusting their hyper-parameters with real data), and complemented by uncertainty propagation models. Such adaptations and extensions are at the core of the NEXT project; hyper-parameter tuning is also a challenge regarding the development plans of the local grids, that heavily rely on graph optimization algorithms.
Furthermore, predictive models of local grids are based on the estimated consumption of end-customers: Linky meters provide coarse grain information only due to privacy issues, and very few samples of fine-grained consumption are available (from volunteer customers). A first task is to transfer knowledge from small data to the whole domain of application. A second task is to directly predict the peak of consumption based on the user cluster profiles and their representativity (see Section 7.4.2).

Another research direction formulates security maintenance as a reinforcement problem, taking inspiration from the recent successes of Deep Reinforcement Learning. This direction is being investigated in Balthazar Donon's RTE CIFRE PhD with RTE (started Oct. 2018).

4.3. Data-driven Numerical Modeling

Participants: Guillaume Charpiat, Cécile Germain, Isabelle Guyon, Flora Jay, Marc Schoenauer, Michèle Sebag
PhD and Post-doc: Victor Estrade, Loris Felardo, Adrian Pol, Théophile Sanchez
Collaboration: D. Rousseau (LAL), M. Pierini (CERN)

As said (section 3.2), in domains where both first principle-based models and equations, and empirical or simulated data are available, their combined usage can support more accurate modelling and prediction, and when appropriate, optimization, control and design. This section describes such applications, with the goal of improving the time-to-design chain through fast interactions between the simulation, optimization, control and design stages. The expected advances regard: i) the quality of the models or simulators (through data assimilation, e.g. coupling first principles and data, or repairing/extending closed-form models); ii) the exploitation of data derived from different distributions and/or related phenomenons; and, most interestingly, iii) the task of optimal design and the assessment of the resulting designs.

The proposed approaches are based on generative and adversarial modelling [116], [102], extending both the generator and the discriminator modules to take advantage of the domain knowledge.

A first challenge regards the design of the model space, and the architecture used to enforce the known domain properties (symmetries, invariance operators, temporal structures). When appropriate, data from different distributions (e.g. simulated vs real-world data) will be reconciled, for instance taking inspiration from real-valued non-volume preserving transformations [84] in order to preserve the natural interpretation.
Another challenge regards the validation of the models and solutions of the optimal design problems. The more flexible the models, the more intensive the validation must be, 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.

CQFD Project-Team

4. Application Domains

4.1. Dependability and safety

Our abilities in probability and statistics apply naturally to industry, in particular in studies of dependability and safety. An illustrative example is the collaboration that started in September 2014 with with THALES Optronique. The goal of this project is the optimization of the maintenance of an onboard system equipped with a HUMS (Health Unit Monitoring Systems). The physical system under consideration is modeled by a piecewise deterministic Markov process. In the context of impulse control, we propose a dynamic maintenance policy, adapted to the state of the system and taking into account both random failures and those related to the degradation phenomenon.

The spectrum of applications of the topics that the team can address is large and can concern many other fields. Indeed non parametric and semi-parametric regression methods can be used in biometry, econometrics or engineering for instance. Gene selection from microarray data and text categorization are two typical application domains of dimension reduction among others. We had for instance the opportunity via the scientific program PRIMEQUAL to work on air quality data and to use dimension reduction techniques as principal component analysis (PCA) or positive matrix factorization (PMF) for pollution sources identification and quantization.

MATHRISK Project-Team

4. Application Domains

4.1. Financial Mathematics, Insurance

The domains of application are quantitative finance and insurance with emphasis on risk modeling and control. In particular, Mathrisk focuses on dependence modeling, systemic risk, market microstructure modeling and risk measures.

SIMSMART Team

4. Application Domains

4.1. Domain 1 – Computational Physics

The development of large-scale computing facilities has enabled simulations of systems at the *atomistic scale* on a daily basis. The aim of these simulations is to bridge the time and space scales between the macroscopic properties of matter and the stochastic atomistic description. Typically, such simulations are based on the ordinary differential equations of classical mechanics supplemented with a random perturbation modeling temperature, or collisions between particles.

Let us give a few examples. In bio-chemistry, such simulations are key to predict the influence of a ligand on the behavior of a protein, with applications to drug design. The computer can thus be used as a *numerical microscope* in order to access data that would be very difficult and costly to obtain experimentally. In that case, a rare event (Objective 1) is given by a macroscopic system change such as a conformation change of the protein. In nuclear safety, such simulations are key to predict the transport of neutrons in nuclear plants, with application to assessing aging of concrete. In that case, a rare event is given by a high energy neutron impacting concrete containment structures.

A typical model used in molecular dynamics simulation of open systems at given temperature is a stochastic differential equation of Langevin type. The large time behavior of such systems is typically characterized by a hopping dynamics between 'metastable' configurations, usually defined by local minima of a potential energy. In order to bridge the time and space scales between the atomistic level and the macroscopic level, specific algorithms enforcing the realization of rare events have been developed. For instance, splitting particle methods (Objective 1) have become popular within the computational physics community only within the last few years, partially as a consequence of interactions between physicists and Inria mathematicians in ASPI (parent of SIMSMART) and MATHERIALS project-teams.

4.2. Domain 2 – Meteorology

The traditional trend in data assimilation in geophysical sciences (climate, meteorology) is to use as prior information some very complex deterministic models formulated in terms of fluid dynamics and reflecting as much as possible the underlying physical phenomenon (see *e.g.*https://www.metoffice.gov.uk/research/modelling-systems/unified-model/). Weather/climate forecasting can then be recast in terms of a Bayesian filtering problem (see Objective 2) using weather observations collected *in situ*.

The main issue is therefore to perform such Bayesian estimations with very expensive infinite dimensional prior models, and observations in large dimension. The use of some linear assumption in prior models (Kalman filtering) to filter non-linear hydrodynamical phenomena is the state-of-the-art approach, and a current field of research, but is plagued with intractable instabilities.

This context motivates two research trends: (i) the introduction of non-parametric, model-free prior dynamics constructed from a large amount of past, recorded real weather data; and (ii) the development of appropriate non-linear filtering approaches (Objective 2 and Objective 3).

SIMSMART will also test its new methods on multi-source data collected in North-Atlantic paying particular attention to coastal areas (*e.g.* within the inter-Labex SEACS).

TOSCA Project-Team

4. Application Domains

4.1. Domain 1

TOSCA is interested in developing stochastic models and probabilistic numerical methods. Our present motivations come from models with singular coefficients, with applications in Geophysics, Molecular Dynamics and Neurosciences; Lagrangian modeling in Fluid Dynamics and Meteorology; Population Dynamics, Evolution and Genetics; Neurosciences; and Financial Mathematics.

4.1.1. Stochastic models with singular coefficients: Analysis and simulation

Stochastic differential equations with discontinuous coefficients arise in Geophysics, Chemistry, Molecular Dynamics, Neurosciences, Oceanography, etc. In particular, they model changes of diffusion of fluids, or diffractions of particles, along interfaces.

For practioners in these fields, Monte Carlo methods are popular as they are easy to interpret — one follows particles — and are in general easy to set up. However, dealing with discontinuities presents many numerical and theoretical challenges. Despite its important applications, ranging from brain imaging to reservoir simulation, very few teams in mathematics worldwide are currently working in this area. The Tosca project-team has tackled related problems for several years providing rigorous approach. Based on stochastic analysis as well as interacting with researchers in other fields, we developed new theoretical and numerical approaches for extreme cases such as Markov processes whose generators are of divergence form with discontinuous diffusion coefficient.

The numerical approximation of singular stochastic processes can be combined with backward stochastic differential equations (BSDEs) or branching diffusions to obtain Monte Carlo methods for quasi-linear PDEs with discontinuous coefficients. The theory of BSDEs has been extensively developed since the 1980s, but the general assumptions for their existence can be quite restrictive. Although the probabilistic interpretation of quasi-linear PDEs with branching diffusions has been known for a long time, there have been only a few works on the related numerical methods.

Another motivation to consider stochastic dynamics in a discontinuous setting came to us from time evolution of fragmentation and coagulation phenomena, with the objective to elaborate stochastic models for the avalanche formation of soils, snow, granular materials or other geomaterials. Most of the models and numerical methods for avalanches are deterministic and involve a wide variety of physical parameters such as the density of the snow, the yield, the friction coefficient, the pressure, the basal topography, etc. One of these methods consists in studying the safety factor (or limit load) problem, related to the shallow flow of a visco-plastic fluid/solid with heterogeneous thickness over complex basal topography. The resulting nonlinear partial differential equation of this last theory involves many singularities, which motivates us to develop an alternative stochastic approach based on our past works on coagulation and fragmentation. Our approach consists in studying the evolution of the size of a typical particle in a particle system which fragments in time.

4.1.2. Stochastic Lagrangian modeling in Computational Fluid Dynamics

Stochastic Lagrangian models were introduced in the eighties to simulate complex turbulent flows, particularly two-phase flows. In Computational Fluid Dynamics (CFD), they are intensively used in the so-called Probability Density Functions (PDF) methods in order to model and compute the reaction-phase terms in the fundamental equations of fluid motions. The PDF methods are currently developed in various laboratories by specialists in scientific computation and physicists. However, to our knowledge, we are innovating in two ways:

- our theoretical studies are the pioneering mathematical analysis of Lagrangian stochastic models in CFD;
- our work on the Stochastic Downscaling Method (SDM) for wind simulation is the first attempt to solve the fundamental equations themselves by a fully 3D stochastic particle method.

We emphasize that our numerical analysis is essential to the SDM development which takes benefits from our deep expertise on numerical schemes for McKean-Vlasov-non-linear SDEs.

4.1.3. Population Dynamics, Evolution and Genetics

The activity of the team on stochastic modeling in population dynamics and genetics mainly concerns application in adaptive dynamics, a branch of evolutionary biology studying the interplay between ecology and evolution, ecological modeling, population genetics in growing populations, and stochastic control of population dynamics, with applications to cancer growth modeling. Stochastic modeling in these areas mainly considers individual-based models, where the birth and death of each individual is described. This class of model is well-developed in Biology, but their mathematical analysis is still fragmentary. Another important topic in population dynamics is the study of populations conditioned to non-extinction, and of the corresponding stationary distributions, called quasi-stationary distributions (QSD). This domain has been the object of a lot of studies since the 1960's, but we made recently significant progresses on the questions of existence, convergence and numerical approximation of QSDs using probabilistic tools rather than the usual spectral tools.

Our activity in population dynamics also involves a fully new research project on cancer modeling at the cellular level by means of branching processes. In 2010 the International Society for Protons Dynamics in Cancer was launched in order to create a critical mass of scientists engaged in research activities on Proton Dynamics in Cancer, leading to the facilitation of international collaboration and translation of research to clinical development. Actually, a new branch of research on cancer evolution is developing intensively; it aims in particular to understand the role of proteins acting on cancerous cells' acidity, their effects on glycolysis and hypoxia, and the benefits one can expect from controlling pH regulators in view of proposing new therapies.

4.1.4. Stochastic modeling in Neuroscience

It is generally accepted that many different neural processes that take place in the brain involve noise. Indeed, one typically observes experimentally underlying variability in the spiking times of an individual neuron in response to an unchanging stimulus, while a predictable overall picture emerges if one instead looks at the average spiking time over a whole group of neurons. Sources of noise that are of interest include ionic currents crossing the neural membrane, synaptic noise, and the global effect of the external environment (such as other parts of the brain).

It is likely that these stochastic components play an important role in the function of both the neurons and the networks they form. The characterization of the noise in the brain, its consequences at a functional level and its role at both a microscopic (individual neuron) level and macroscopic level (network of thousands of neurons) is therefore an important step towards understanding the nervous system.

To this end, a large amount of current research in the neuroscientific literature has involved the addition of noise to classical purely deterministic equations resulting in new phenomena being observed. The aim of the project is thus to rigorously study these new equations in order to be able to shed more light on the systems they describe.

4.1.5. Stochastic modeling in Financial Mathematics

4.1.5.1. Technical Analysis

In the financial industry, there are three main approaches to investment: the fundamental approach, where strategies are based on fundamental economic principles; the technical analysis approach, where strategies are based on past price behavior; and the mathematical approach where strategies are based on mathematical models and studies. The main advantage of technical analysis is that it avoids model specification, and thus calibration problems, misspecification risks, etc. On the other hand, technical analysis techniques have limited theoretical justifications, and therefore no one can assert that they are risk-less, or even efficient.

4.1.5.2. Financial Risks Estimation and Hedging

Popular models in financial mathematics usually assume that markets are perfectly liquid. In particular, each trader can buy or sell the amount of assets he/she wants at the same price (the “market price”). They moreover assume that the decision taken by the trader does not affect the price of the asset (the small investor assumption). In practice, the assumption of perfect liquidity is never satisfied but the error due to liquidity is generally negligible with respect to other sources of error such as model error or calibration error, etc.

Derivatives of interest rates are singular for at least two reasons: firstly the underlying (interest rate) is not directly exchangeable, and secondly the liquidity costs usually used to hedge interest rate derivatives have large variation in times.

Due to recurrent crises, the problem of risk estimation is now a crucial issue in finance. Regulations have been enforced (Basel Committee II). Most asset management software products on the markets merely provide basic measures (VaR, Tracking error, volatility) and basic risk explanation features (e.g., “top contributors” to risk, sector analysis, etc).

4.1.5.3. Energy and Carbon Markets

With the rise of renewable energy generation (from solar, wind, waves...), engineers face new challenges which heavily rely on stochastic and statistical problems.

Besides, in the context of the beginning of the second phase (the Kyoto phase) in 2008 of the European carbon market, together with the fact that French carbon tax was scheduled to come into law on Jan. 1, 2010, the year 2009 was a key year for the carbon price modeling. Our research approach adopts the point of view of the legislator and energy producers. We used both financial mathematical tools and a game theory approach. Today, with the third phase of the EU-ETS, that didn’t yet start, and the report form the Cour des Comptes (October 2013) that pointed out (among many others point) the lack of mathematical modeling on such carbon market design, we continue our research in this direction.

4.1.5.4. Optimal Stopping Problems

The theory of optimal stopping is concerned with the problem of taking a decision at the best time, in order to maximise an expected reward (or minimise an expected cost). We work on the general problem of optimal stopping with random discounting and additional cost of observation.

4.1.5.5. First hitting times distributions

Diffusion hitting times are of great interest in finance (a typical example is the study of barrier options) and also in Geophysics and Neurosciences. On the one hand, analytic expressions for hitting time densities are well known and studied only in some very particular situations (essentially in Brownian contexts). On the other hand, the study of the approximation of the hitting times for stochastic differential equtions is an active area of research since very few results still are available in the literature.