



RESEARCH CENTER

FIELD

**Applied Mathematics, Computation  
and Simulation**

Activity Report 2015

# Section Application Domains

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## ACUMES Team

# 4. Application Domains

## 4.1. Active flow control for transportation systems

The reduction of CO<sub>2</sub> 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 [142]. 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 [98]. 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. Performance optimization in water sports

Phenomena encountered in water sports provide challenging modeling and optimization problems. Complex flows are usually considered in this context, including turbulence with strong unsteadiness effects and free surface. These problems can be multi-physic, for instance the simulation of a sail behavior requires to solve a fluid-structure interaction problem. Moreover, from an optimization point of view, a delicate compromise between performance and robustness with respect to the uncertain environment is usually sought. Nevertheless, a significant improvement of the performance can be achieved in this area, for which the use of simulation and optimization methods is just beginning. In this context, we are working with specialists of different disciplines (racing kayak and yachting) to develop specific optimization strategies. In particular, the use of meta-modeling techniques, able to aggregate simulations of different accuracies, is studied, as well as robust optimization formulations to account for uncertainties.

## 4.3. Concurrent design for building systems

The lifetime of a building goes through three stages: construction, use and destruction. To each of these phases correspond quality criteria related in particular to:

- Safety: structural, fire, evacuation, chemical spread, etc.
- Well-being of its occupants: thermal and acoustic comfort.
- Functionality of its intended use.
- Environmental impact.

These stages and criteria form a complex system, the so-called building system, whose overall quality (in an intuitive sense) is directly impacted by many factors, very heterogeneous, such as the geographical location or the shape or material composition of some of its components (windows, frames, thermal convectors positions, etc.) It is obvious that the optimization process of these settings must be performed at the "zero" stage of the project design. Moreover, the optimization process has to follow a global approach, taking into account all the concurrent criteria that intervene in the design of building systems.

The application of up-to-date concurrent optimization machinery (games, Pareto Fronts) for multiphysics systems involved in the building is an original approach. With our industrial partner, who wishes routine use of new high performance components in the construction of buildings, we expect that our approach will yield breakthrough building performances (with respect to the above criteria) compared to the current standards.

The research project relies on the ADT BuildingSmart (see software development section) for the implementation of industrial standard software demonstrators.

#### 4.4. 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 [103]. Further improvements require more advanced models, keeping into better account interactions at the microscopic scale, and adapted control techniques, see [57] 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 [70], [96], 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 [107].
- *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 [105] 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 [64], [65]), with a stress on the (fixed) Eulerian framework. Up to our knowledge, they have not been studied 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 [78], [97] or via the Hamilton-Jacobi approach [64], [65] could allow to optimize the flow by controlling some specific vehicles corresponding to internal conditions.

## 4.5. 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.

The cells in epithelial sheets (monolayers) maintain strong cell-cell contact during their collective migration. Although it is well known that under some experimental conditions apical and basal sites play distinctive important roles during the migration, as well as the substrate itself [130], we consider here biological experiments where the apico-basal polarization does not take place. Thus, the cell monolayer can be considered as a 2 dimensional continuous structure. These epithelial monolayers, as the Madin-Darby Canine Kidney (MDCK) cells [53], [90], are universally used as multicellular models to study the migratory 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 [101], 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 [89] it is shown that MDCK cells extend cryptic lamellipodia to drive the migration, several rows behind the wound edge. In [125] 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 interaction of the cells (at the cell-cell level, including the F-actin, but not e.g. the migration-related protein scale). 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 [87], [92], [94].

## 4.6. 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
- nanaphotonic 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.

This research activity is aimed to make our methodologies and application fields more diverse, and we expect to be confronted to novel optimization problematics raised by the specific context.

## **CAGIRE Team**

# **4. Application Domains**

## **4.1. Aeronautical combustion chambers**

The combustion chamber of aeronautical engines is the system of practical interest we are interested in as far as propulsion devices are concerned. The MAVERIC test facility was developed by P. Bruel in that framework during the theses (CIFRE Turbomeca) of A. Most (2007) and J.-L. Florenciano (2013). The initial objective was to reproduce experimentally a simplified flow configuration (jet(s) in crossflow) representative of that encountered at the level of the effusion cooled aeronautical combustion chambers walls. The experimental data were used by Safran/Turbomeca to assess the predictive capability of LES simulations during our joint participation in the EU-FP7 KIAI program (2009-2013). Concerning DNS, the jet in crossflow configurations of our AeroSol based simulations which represent our contribution to the EU IMPACT-AE program (2011-2016) were chosen in partnership with Turbomeca who is leading the corresponding work package. Last but not least, tests aimed at demonstrating the feasibility of characterizing in situ by PIV the velocity field of flows emerging from different kinds of fuel nozzles were carried out at the Turbomeca premises in 2012 and 2013. Although our main present industrial partners are large companies, we are and will be actively targeting much smaller companies (SMEs) especially in the southwest part of France. In that respect, the partnership we just started with AD Industries which is manufacturing fuel nozzles as well as combustion chambers for business jet engines is emblematic of our involvement in such kind of partnership.

## **4.2. Power stations**

The cooling of key components of power stations in case of emergency stops is a critical issue. R. Manceau has established a long term collaboration (4 PhD thesis) 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, in order to improve the physical description of the complex interaction phenomena involved in such applications. In the framework of the co-supervision of the PhD thesis (CIFRE EDF) of J.-F. Wald, strategies are developed to adapt the EB-RSM turbulence model to a local modification of the scale of description of the flow in the near-wall region: refined scale (fine mesh in the near-wall region) or coarse scale (with wall functions). Indeed, the complexity of the industrial geometries is such that a fine mesh along solid boundaries in the whole system is usually not possible/desirable.



## CARDAMOM 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 immersed boundary capturing of moving ice debris, whose movements are computed using basic mechanical laws.

In [75] 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 [65], [122]. In these methods we compensate for the error at solid walls introduced by the penalization by using anisotropic mesh adaptation [94], [113], [114]. 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 [77]. 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 [79], [74] 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 [125], 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 [144], 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 accommodation 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 accommodation 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 [78], [117]. 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 [124] 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 using 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

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

where  $\rho$  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,  $\Gamma$  may be lower than 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  $\Gamma \ll 1$ , 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 [87]). 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 [143], 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 [98], 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 anisotropic 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 [98], asymptotic models for 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 [128].

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 with 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 for the transport equations (Fick's laws) with chemical reactions sources, plus a potential model for the flow of oxide [90], [95], [126]. 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 (see e.g. [86]) 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 [110], [132], [123], [92], to hybrid methods coupling dispersive PDEs with hyperbolic ones, and trying to mimic wave breaking with travelling bores [136], [137], [135], [107], [100]. 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 investigated, 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 [76].

## **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 build 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 from 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 grayscale 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, and 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 is 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 showing 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 coefficient  $D$  will appear as the slope of the semi-log plot of the signal (in appropriate 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.

## 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,
- 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 output criterion with respect to all the 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.

One particular case of inverse problems is *data assimilation* [32] 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 through AD [35]. Figure 1 shows an example of a data assimilation exercise using the oceanography code OPA [33] and its AD-adjoint produced by Tapenade.

The special case of *4Dvar* data assimilation is particularly challenging. The 4<sup>th</sup> 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.

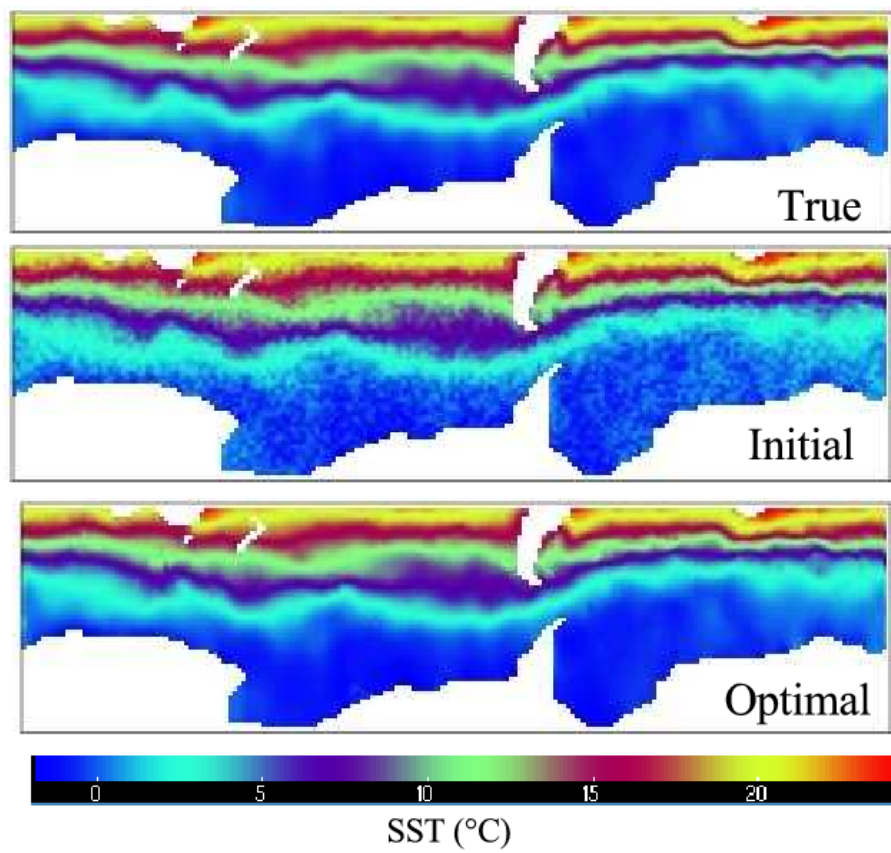


Figure 1. Twin experiment using the adjoint of OPA. Random noise, added to a simulation of the sea surface temperature around the Antarctic, is removed by minimizing the discrepancy with the physical model

#### 4.4. Linearization

Simulating a complex system often requires solving a system of Partial Differential Equations. This can be too expensive, in particular in the context of real time. 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.

**GAMMA3 Project-Team (section vide)**

**IPSO Project-Team (section vide)**

## MATHERIALS Project-Team

# 4. Application Domains

## 4.1. Homogenization and related problems

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

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

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

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

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

## 4.2. Electronic structure of large systems

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

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

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

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

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

## 4.3. Computational Statistical Mechanics

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

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

For practical numerical computations of matter at the microscopic level, following the dynamics of every atom would require simulating  $\mathcal{N}_A$  atoms and performing  $O(10^{15})$  time integration steps, which is of course impossible! These numbers should be compared with the current orders of magnitude of the problems that can be tackled with classical molecular simulation, where several millions of atoms only can be followed over time scales of the order of 0.1  $\mu$ s.



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

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

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

Another major aim of molecular simulation, maybe even more important than the previous one, is to compute macroscopic quantities or thermodynamic properties, typically through averages of some functionals of the system. In this case, molecular simulation is a way to obtain *quantitative* information on a system, instead of resorting to approximate theories, constructed for simplified models, and giving only qualitative answers. Sometimes, these properties are accessible through experiments, but in some cases only numerical computations are possible since experiments may be unfeasible or too costly (for instance, when high pressure or large temperature regimes are considered, or when studying materials not yet synthesized). More generally, molecular simulation is a tool to explore the links between the microscopic and macroscopic properties of a material, allowing one to address modelling questions such as “Which microscopic ingredients are necessary (and which are not) to observe a given macroscopic behavior?”

## MEMPHIS Team

# 4. Application Domains

## 4.1. Energy conversion

We consider applications in the domain of wind engineering and sea-wave converters. As an example of application of our methods, we show a recent realisation where we model a sea-wave energy converter, see figure 1. In this unsteady example, the full interaction between the rigid floater, air and water is described by a monolithic model, the Newton's law, where physical parameters 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. The background method for fluid structure interface is the volume penalization method where the level set functions is used to improve the degree of accuracy of the method and also to follow the object. The simulations are unsteady, three dimensional, with  $O(10^8)$  grid points on 512 CPUs.

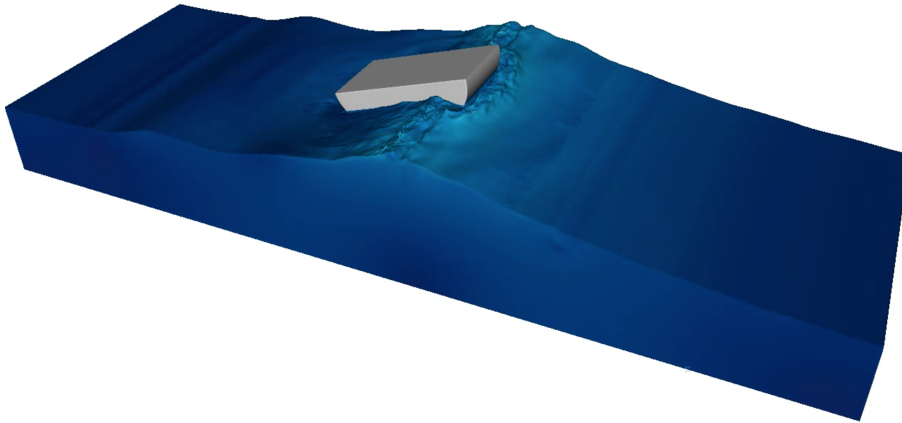


Figure 1. Numerical modeling of a sea-wave converter by a monolithic model and Cartesian meshes.

## 4.2. Impacts

We study hyper-velocity phenomena where several materials are involved. An example of this approach is the impact of a projectile immersed in air over a shield, see figure 2. Using the same set of equations across the entire domain, we model the compressible fluid, the hyperelastic material and the interaction at the interface that models possible rebounds. Only the constitutive laws characterize the different materials.

The simulation is performed over a  $4000^2$  fixed Cartesian grid so that the resulting numerical scheme allows an efficient parallelization (512 processors in this case) with an isomorphism between grid partitioning and processor topology. The challenge for our team is to increase the accuracy of the simulation thanks to grid refinement in the vicinity of the moving interfaces, still guaranteeing scalability and a simple computational set up.

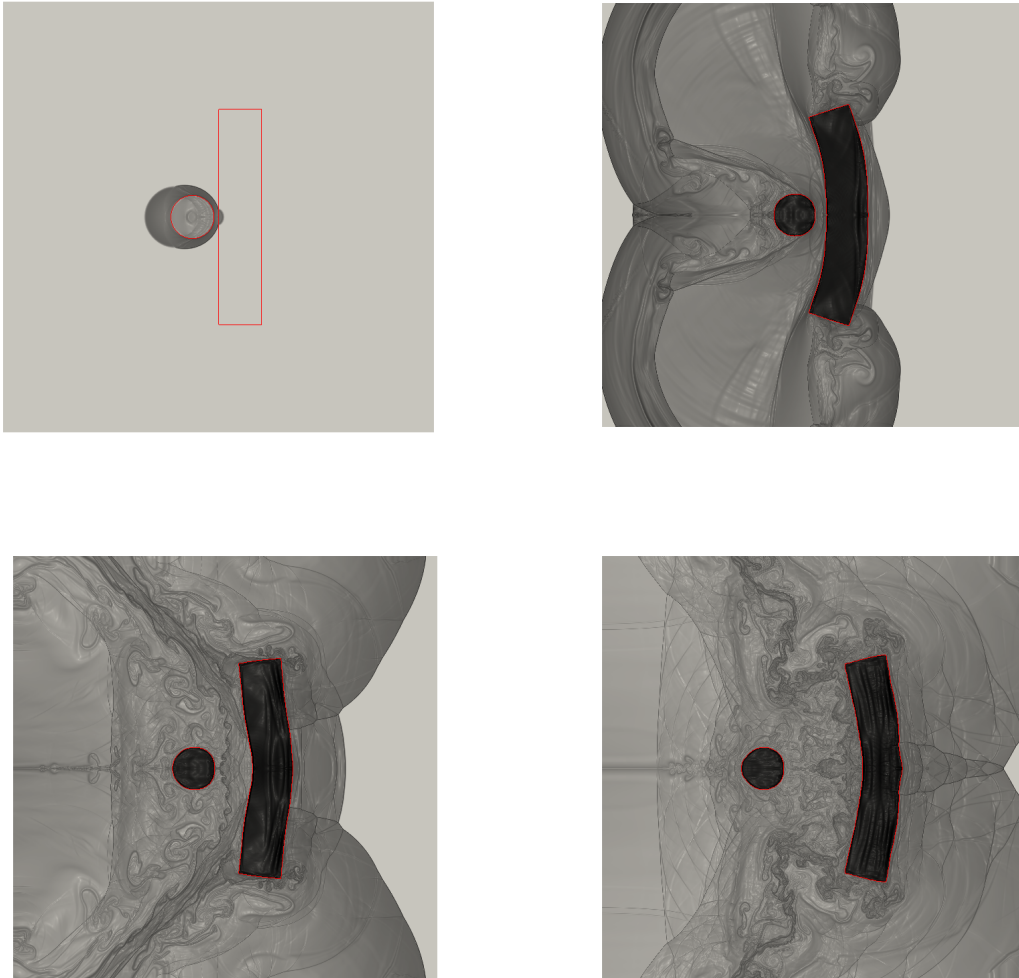
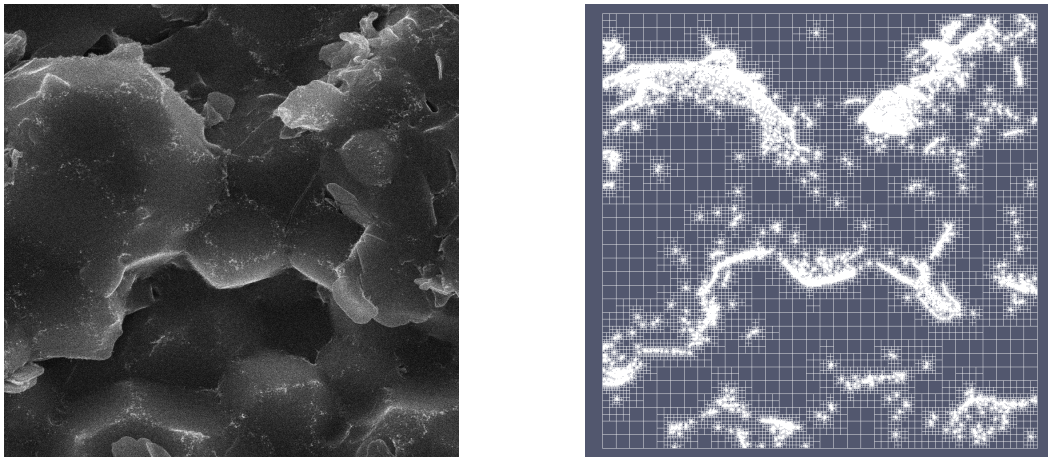


Figure 2. Impact and rebound of a copper projectile on a copper plate. Interface and schlieren at  $50\mu\text{s}$ ,  $199\mu\text{s}$ ,  $398\mu\text{s}$  and  $710\mu\text{s}$ . From left to right, top to bottom.

### 4.3. New materials

Thanks to the multiscale schemes that we develop, we can characterize new materials from constituents. As an example, consider the material presented in figure 3 left. It is a picture of a dry foam that is used as dielectric material. This micrography is taken at the scale of the dry bubbles, where on the surface of the bubble one can observe the carbon nanotubes as white filaments. The presence of nanotubes in the dry emulsion makes the electrical capacitance of this material significantly affected by its strain state by creating aligned dipoles at a larger scale compared to the size of the dielectric molecules. It is a typical multi-scale phenomenon in presence of widely varying physical properties. This material is used to generate micro currents when it undergoes vibrations. The schemes that we devise allow to model this multi-scale irregular material by a monolithic model (same equation in the whole domain), in this case a variable coefficient diffusion equation. In order to recover adequate accuracy, the numerical scheme is adapted near the interfaces between the different subdomains. The computational hierarchical mesh is directly derived by the micrography of the material (figure 3 right).



*Figure 3. A micrography of an electrostrictive material is shown on the left: the bright regions visualize the carbon nanotubes. The hierarchical grid adapted to the nanotubes is shown on the right. The ratio between the largest and the smallest cell side is  $2^7$ . Project developed in collaboration with the CRPP physics and chemistry lab of the CNRS in Bordeaux (Annie Colin, Philippe Poulin).*

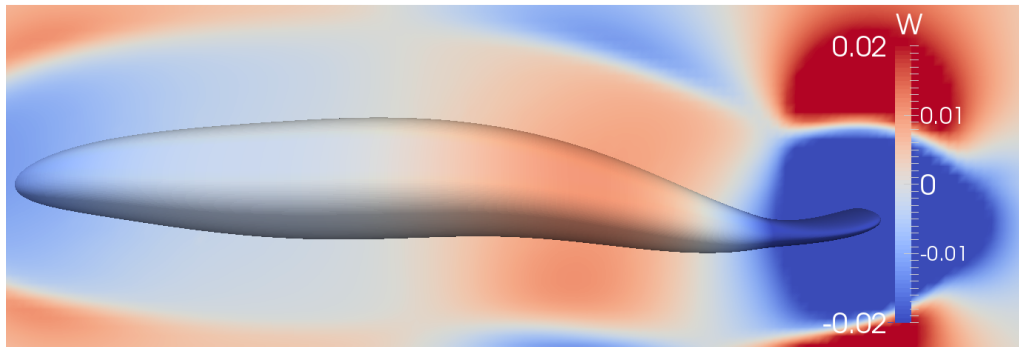
### 4.4. Bio-inspired robotic swimming

In bioinspired robotic swimming the aim is of simulating a three-dimensional swimmer starting from pictures. The first step is to build the three-dimensional fish profile based on two-dimensional data retrieved from the picture of an undeformed fish at rest. This is done by a skeleton technique and a three-dimensional level set function describing the body surface. Then the skeleton is deformed using an appropriate swimming law to obtain a sequence of level set functions corresponding to snapshots of the body surface uniformly taken at different instants.

Thanks to skeleton deformation we typically reconstruct 20% of the snapshots necessary to simulate a swimming stroke, since the time scale of the simulation is significantly smaller than the time step between two subsequent reconstructed snapshots. Also, the surface deformation velocity is required to set the boundary conditions of the flow problem. For this reason it is necessary to build intermediate level set functions and to compute the deformation velocity field between subsequent fish snapshots. Optimal transportation is well

suited to achieve this goal providing an objective model to compute intermediate geometries and deformation velocities.

Numerical simulations have been performed in 3D, see figure 4 . However, it has been observed that these algorithms do not preserve the physics/features of the represented objects. Indeed, the fish tends to compress during the deformation.



*Figure 4. Comparison of the exact deformation velocity (presented inside the swimmer) and the approximated velocity identified using optimal transport (represented outside the fish). The error of the identification scheme is negligible for this component of the velocity, as it can be inferred by comparing the two velocities on the boundary of the swimmer.*

For this reason, we will consider incompressible or rigid transports.

## MEPHYSTO Team

# 4. Application Domains

## 4.1. Mechanics of heterogeneous media

The mechanics of heterogeneous materials aims at characterizing the macroscopic properties of heterogeneous materials using the properties of their constituents.

The homogenization theory is a natural tool for this task. In particular, for linear problems (linear conductivity or linear elasticity), the macroscopic properties are encoded into a single (conductivity or elasticity) homogenized tensor. The numerical approximation of this homogenized tensor is a typical objective of quantitative homogenization.

For nonlinear problems, such as rubber elasticity, the macroscopic properties are no longer characterized by a single tensor, but rather by a nonlinear energy density. Our aim is to relate qualitatively and quantitatively the (precise but unpractical) statistical physics picture to explicit macroscopic constitutive laws that can be used for practical purposes. This endeavor is relevant both in science and technology. The rigorous derivation of rubber elasticity from polymer-physics was indeed emphasized by John Ball as an important open problem of nonlinear elasticity in his survey [44] on the field. Its solution could shed light on some aspects of polymer-physics. The associated ab initio derivation of constitutive laws (as an alternative to phenomenological laws) would also be of interest to computational mechanics and rubber industry.

For this application domain, we work in close collaboration with physicists (François Lequeux, ESPCI) and researchers from mechanics and computational mechanics (Patrick Le Tallec, Ecole polytechnique).

## 4.2. Numerical simulation in heterogeneous media

Solving numerically PDEs in highly heterogeneous media is a problem encountered in many situations, such as the transport of pollutants or the design of oil extraction strategies in geological undergrounds. When such problems are discretized by standard numerical methods the number of degrees of freedom may become prohibitive in practice, whence the need for other strategies.

Numerical solution methods inspired by asymptotic analysis are among the very few feasible alternatives, and started fifteen years ago with the contributions of Hou and Wu [59], Arbogast [40] etc. We refer to [54], [70], [3] for a recent state of the art. Numerical homogenization methods usually amount to looking for the solution of the problem (1) in the form  $u_\varepsilon(x) \simeq u_0(x) + \varepsilon \nabla u_0(x) \cdot \Phi(x, \frac{x}{\varepsilon})$ , where  $\Phi$  is a proxy for the corrector field computed locally at point  $x$  (in particular, one does not use explicitly that the problem is periodic so that the method can be used for more general coefficients) and  $u_0$  is a function which does not oscillate at scale.

Relying on our quantitative insight in stochastic homogenization, a first task consists in addressing the three following prototypical academic examples: periodic, quasi-periodic, and stationary ergodic coefficients with short range dependence. The more ambitious challenge is to address more complex coefficients (of interest to practitioners), and design adaptive and efficient algorithms for diffusion in heterogeneous media.

## 4.3. Laser physics

Our contribution to the analysis of models in laser physics is motivated by the LabEx CEMPI (Centre Européen pour les Mathématiques, la Physique et leurs Interactions, a large eight-year research and training project approved by the French government in February 2012 as a "Laboratoire d'Excellence" and an initiative of mathematicians and physicists of the Université Lille 1). For this application domain, we work in close collaboration with physicists, which ensures our direct impact on these scientific issues. We focus on two applications: optical fibers and cold atoms.

In collaboration with physicists from the PhLAM laboratory in Lille, we aim at developing new techniques for the numerical integration of a family of 1D Schrödinger-like equations modelling the propagation of laser pulses in optical fibers. The questions arising are challenging since physicists would like to have fairly fast and cheap methods for their problems, with correct qualitative and quantitative behaviors. Another point is that they are interested in methods and codes that are able to handle different physical situations, hence different terms in the NLS equation. To meet these requirements, we will have to use numerical time-integration techniques such as splitting methods or exponential Runge-Kutta methods, space discretization techniques such as finite differences and fast Fourier transforms, and absorbent boundary conditions. Our goal, together with the physicists is to be able to reproduce numerically the results of the experiments they make in actual optical fibers, and then to be able to tune parameters numerically to get more insight into the appearance of rogue waves beyond the dispersive blowup phenomenon.

Recall that the Schrödinger equation also describes Bose-Einstein condensates. A second experimental team at PhLAM projects to study questions related to Anderson localization in such condensates. In fact, they will realize the "kicked rotor" (see [51]), which provides a paradigm for Anderson localization, in a Bose-Einstein condensate. We plan to collaborate with them on the theoretical underpinnings of their findings, which pose many challenging questions.

## MOKAPLAN Project-Team

# 4. Application Domains

## 4.1. Freeform Optics

Following the pioneering work of Caffarelli and Oliker [88], Wang [182] has shown that the inverse problem of freeforming a *convex* reflector which sends a prescribed source to a target intensity is a particular instance of Optimal Transportation. This is a promising approach to automatize the industrial design of optimized energy efficient reflectors (car/public lights for instance). We show in figure 10 the experiment setting and one of the first numerical simulations produced by the ADT Mokabajour.

The method developed in [63] has been used by researchers of TU Eindhoven in collaboration with Philips Lighting Labs to compute reflectors [165] in a simplified setting (directional light source). Another approach, based on a geometric discretization of Optimal Transportation has been developed in [8], and is able to handle more realistic conditions (punctual light source).

Solving the exact Optimal Transportation model for the Reflector inverse problem involves a generalized Monge-Ampère problem and is linked to the open problem of  $c$ -convexity compatible discretization we plan to work on. The corresponding software development is the topic of the starting ADT Mokabajour.

### 4.1.1. Software and industrial output.

See section 4.3 below for softwares. These method will clearly become mainstream in reflector design but also in lense design [168]. The industrial problems are mainly on efficiency (light pollution) and security (car head lights) based on free tailoring of the illumination. The figure below is an extreme test case where we exactly reproduce an image. They may represent one of the first incursion on PDE discretization based methods into the field of non-imaging optics.



Figure 10. A constant source to a prescribed image (center). The reflector is computed (but not shown) and a resimulation using ray tracing shows the image reflected by the computed reflector.



## 4.2. Metric learning for natural language processing

The analysis of large scale datasets to perform un-supervised (clustering) and supervised (classification, regression) learning requires the design of advanced models to capture the geometry of the input data. We believe that optimal transport is a key tool to address this problem because (i) many of these datasets are composed of histograms (social network activity, image signatures, etc.) (ii) optimal transport makes use of a ground metric that enhances the performances of classical learning algorithms, as illustrated for instance in [114].

Some of the theoretical and numerical tools developed by our team, most notably Wasserstein barycenters [46], [71], are now becoming mainstream in machine learning [67], [114]. In its simplest (convex) form where one seeks to only maximize pairwise wasserstein distances, metric learning corresponds to the congestion problem studied by G. Carlier and collaborators [102], [74], and we will elaborate on this connection to perform both theoretical analysis and develop numerical schemes (see for instance our previous work [64]).

We aim at developing novel variational estimators extending classification regression energies (SVM, logistic regression [129]) and kernel methods (see [173]). One of the key bottleneck is to design numerical schemes to learn an optimal metric for these purpose, extending the method of Marco Cuturi [113] to large scale and more general estimators. Our main targeted applications is natural language processing. The analysis and processing of large corpus of texts is becoming a key problems at the interface between linguistic and machine learning [50]. Extending classical machine learning methods to this field requires to design suitable metrics over both words and bag-of-words (i.e. histograms). Optimal transport is thus a natural candidate to bring innovative solutions to these problems. In a collaboration with Marco Cuturi (Kyoto University), we aim at unleashing the power of transportation distances by performing ground distance learning on large database of text. This requires to lift previous works on distance on words (see in particular [159]) to distances on bags-of-words using transport and metric learning.



Figure 11. Examples of two histogram (bag-of-words) extracted from the congress speech of US president. In this application, the goal is to infer a meaningful metric on the words of the english language and lift this metric to histogram using OT technics.

## 4.3. Physics

The Brenier interpretation of the generalized solutions of Euler equations in the sense of Arnold is an instance of multi-marginal optimal transportation, a recent and expanding research field which also appears in DFT (see chemistry below). Recent numerical developments in OT provide new means of exploring these class of solutions.

In the years 2000 and after the pioneering works of Otto, the theory of *many-particle systems* has become “geometrized” thanks to the observed intimate relation between the geometric theory of geodesic convexity in the Wasserstein distance and the proof of entropy dissipation inequalities that determine the trend to

equilibrium. The OT approach to the study of equilibration is still an extremely active field, in particular the various recently established connections to sharp functional inequalities and isoperimetric problems.

A third specific topic is the use of optimal transport models in *non-imaging optics*. Light intensity here plays the role of the source/target prescribed mass and the transport map defines the physical shape of specular reflector or refracting lense achieving such a transformation. This models have been around since the works of Oliker and Wang in the 90's. Recent numerical progresses indicate that OT may have an important industrial impact in the design of optical elements and calls for further modelisation and analysis.

#### 4.4. Chemistry

The treatment of *chemical reactions* in the framework of OT is a rather recent development. The classical theory must be extended to deal with the transfer of mass between different particle species by means of chemical reactions. That extension is still far from complete at the moment, but there is a lot of progress currently, some of which we try to capture in the workshop.

A promising and significant recent advance is the introduction and analysis of a novel metric that combines the pure transport elements of the Wasserstein distance with the annihilation and creation of mass, which is a first approximation of chemical reactions. The logical next challenge is the extension of OT concepts to vectorial quantities, which allows to rewrite cross-diffusion systems for the concentration of several chemical species as gradient flows in the associated metric. An example of application is the modeling of a *chemical vapor deposition process*, used for the manufacturing of thin-film solar cells for instance. This leads to a degenerate cross-diffusion equations, whose analysis — without the use of OT theory — is delicate. Finding an appropriate OT framework to give the formal gradient flow structure a rigorous meaning would be a significant advance for the applicability of the theory, also in other contexts, like for biological multi-species diffusion.

A very different application of OT in chemistry is a novel approach to the understanding of *density functional theory* (DFT) by using optimal transport with “Coulomb costs”, which is highly non convex and singular. Albeit this theory shares some properties with the usual optimal transportation problems, it does not induce a metric between probability measures. It also uses the multi-marginal extension of OT, which is an active field on its own right.

#### 4.5. Biology

OT methods have been introduced in biology via gradient flows in the Wasserstein metric. Writing certain *chemotaxis* systems in variational form allowed to prove sharp estimates on the long time asymptotics of the bacterial aggregation. This application had a surprising payback on the theory: it lead to a better understanding and novel proofs of important functional inequalities, like the logarithmic Hardy-Littlewood-Sobolev inequality. Further applications followed, like transport models for species that avoid over-crowding, or cross-diffusion equations for the description of *biologic segregation*. The inclusion of dissipative cross-diffusion systems into the framework of gradient flows in OT-like metrics appears to be one of the main challenges for the future development of the theory. This extension is not only relevant for biological applications, but is clearly of interest to participants with primary interest in physics or chemistry as well.

Further applications include the connection of OT with game theory, following the idea that many selection processes are based on competition. The ansatz is quite universal and has been used in other areas of the *life sciences* as well, like for the modeling of personal income in economics. If time permits, some of those “exotic” applications will be discussed in the workshop as well.

#### 4.6. Medical Imaging

Applications of variational methods are widespread in medical imaging and especially for diffeomorphic image matching. The formulation of large deformation by diffeomorphisms consists in finding geodesics on a group of diffeomorphisms. This can be seen as a non-convex and smoothed version of optimal transport where a correspondence is sought between objects that can be more general than densities. Whereas the

diffeomorphic approach is well established, similarity measures between objects of interest are needed in order to drive the optimization. While being crucial for the final registration results, these similarity measures are often non geometric due to a need of fast computability and gradient computation. However, our team pioneered the use of entropic smoothing for optimal transport which gives fast and differentiable similarity measures that take into account the geometry. Therefore, we expect an important impact on this topic, work still in progress. This example of application belongs to the larger class of inverse problems where a geometric similarity measure such as optimal transport might enhance notably the results. Concerning this particular application, potential interactions with the Inria team ARAMIS and also the team ASCLEPIOS can leverage new proposed similarity measure towards a more applicative impact.

## **4.7. Economics**

Recent years have seen intense cross-fertilization between OT and various problems arising in economics. The principal-agent problem with adverse selection is particularly important in modern microeconomics, mathematically it consists in minimizing a certain integral cost functional among the set of  $c$ -concave functions, this problem is convex under some conditions related to the MTW regularity theory for OT as shown in the important paper [120]. Other examples of fruitful interactions between mathematical economics concern multi-marginal OT and multi-populations matching [98], or games with a continuum of agents and Cournot-Nash equilibria [68]. The team has as strong expertise, both numerical and theoretical in the field of variational problems subject to a convexity constraint and their applications to the principal-agent problem. Our expertise in numerical OT and entropic regularization will also enable us to develop efficient solvers for realistic matching and hedonic pricing models.

## 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 telemedicine, 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 (Finite Difference Time Domain) method due to Yee [62]. 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 [12].

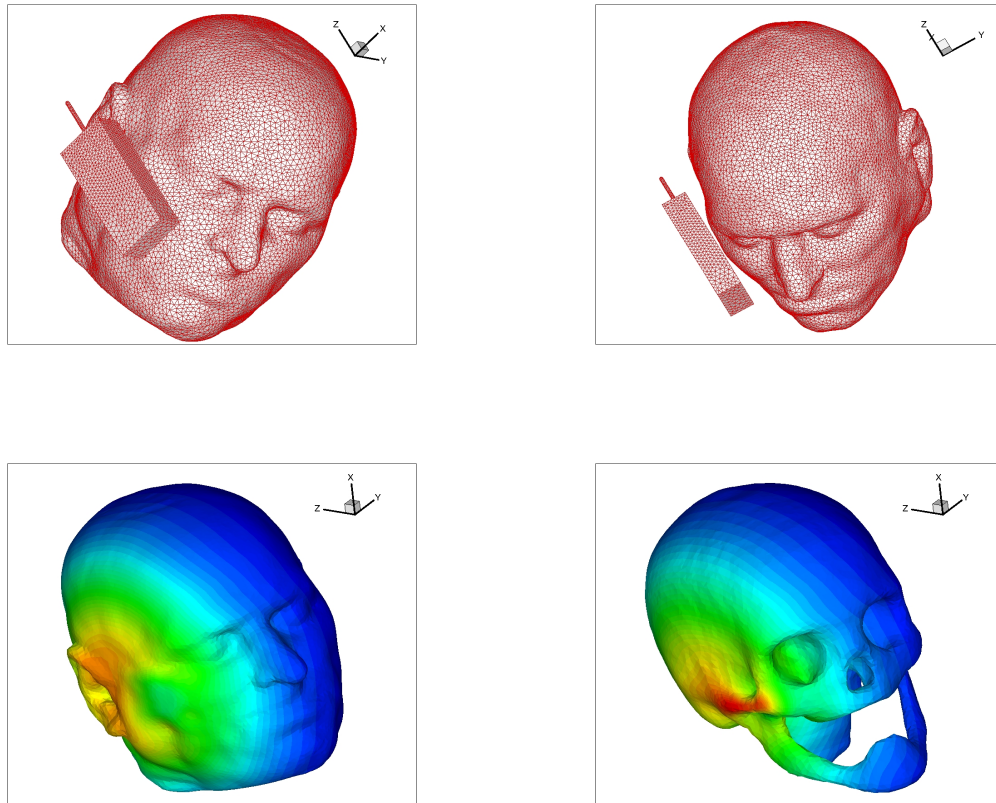


Figure 1. Exposure of head tissues to an electromagnetic wave emitted by a localized source. Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

#### 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 plasmomonic 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 [55]- [63].

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 [60]. 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 [58]- [59]- [53]. 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.

## 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, in particular in the context of 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.

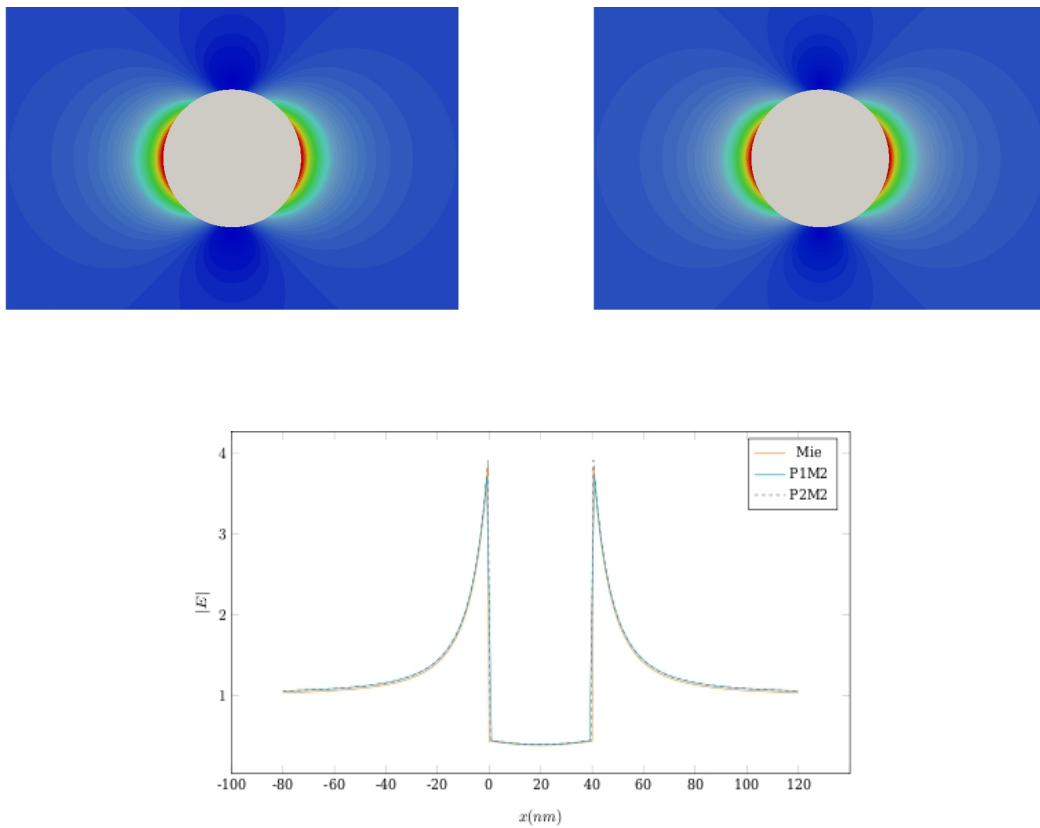


Figure 2. Scattering of a 20 nanometer radius gold nanosphere by a plane wave. The gold properties are described by a Drude dispersion model. Modulus of the electric field in the frequency domain. Top left figure: Mie solution. Top right figure: numerical solution. Bottom figure: 1d plot of the electric field modulus for various orders of approximation.

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 [61] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by Yee [62] 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 initiated a close collaboration with CETE Méditerranée <http://www.cete-mediterranee.fr/gb> which is a regional technical and engineering centre whose activities are concerned with seismic hazard assessment studies, and IFSTTAR <http://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.

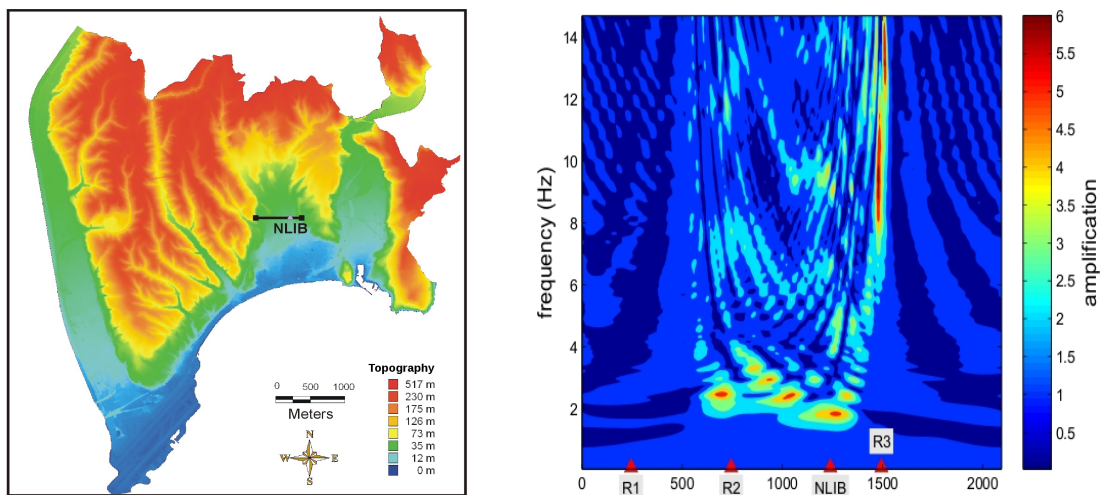


Figure 3. Propagation of a plane wave in a heterogeneous model of Nice area (provided by CETE Méditerranée). Left figure: topography of Nice and location of the cross-section used for numerical simulations (black line). Right figure: transfer functions (amplification) for a vertically incident plane 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.

#### 4.2.2. Seismic exploration

This application topic has been considered recently by the NACHOS project-team and this is done 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 seismic 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

# 4. Application Domains

## 4.1. Overview

NANO-D is *a priori* concerned with all applications domains involving atomistic representations, including chemistry, physics, electronics, material science, biology, etc.

Historically, though, our first applications have been in biology, as the next two sections detail. Thanks to the development of algorithms to efficiently simulate reactive force fields, as well as to perform interactive quantum mechanical calculations, however, we now have the possibility to address problems in chemistry, and physics.

## 4.2. Structural Biology

Structural biology is a branch of molecular biology, biochemistry, and biophysics concerned with the molecular structure of biological macromolecules, especially proteins and nucleic acids. Structural biology studies how these macromolecules acquire the structures they have, and how alterations in their structures affect their function. The methods that structural biologists use to determine the structure typically involve measurements on vast numbers of identical molecules at the same time, such as X-Ray crystallography, NMR, cryo-electron microscopy, etc. In many cases these methods do not directly provide the structural answer, therefore new combinations of methods and modeling techniques are often required to advance further.

We develop a set of tools that help biologists to model structural features and motifs not resolved experimentally and to understand the function of different structural fragments.

- Symmetry is a frequent structural trait in molecular systems. For example, most of the water-soluble and membrane proteins found in living cells are composed of symmetrical subunits, and nearly all structural proteins form long oligomeric chains of identical subunits. Only a limited number of symmetry groups is allowed in crystallography, and thus, in many cases the native macromolecular conformation is not present on high-resolution X-ray structures. Therefore, to understand the realistic macromolecular packing, modeling techniques are required.
- Many biological experiments are rather costly and time-demanding. For instance, the complexity of mutagenesis experiments grows exponentially with the number of mutations tried simultaneously. In other experiments, many candidates are tried to obtain a desired function. For example, about 250,000 candidates were tested for the recently discovered antibiotic Platensimycin. Therefore, there is a vast need in advance modeling techniques that can predict interactions and foresee the function of new structures.
- Structure of many macromolecules is still unknown. For other complexes, it is known only partially. Thus, software tools and new algorithms are needed by biologists to model missing structural fragments or predict the structure of those molecule, where there is no experimental structural information available.

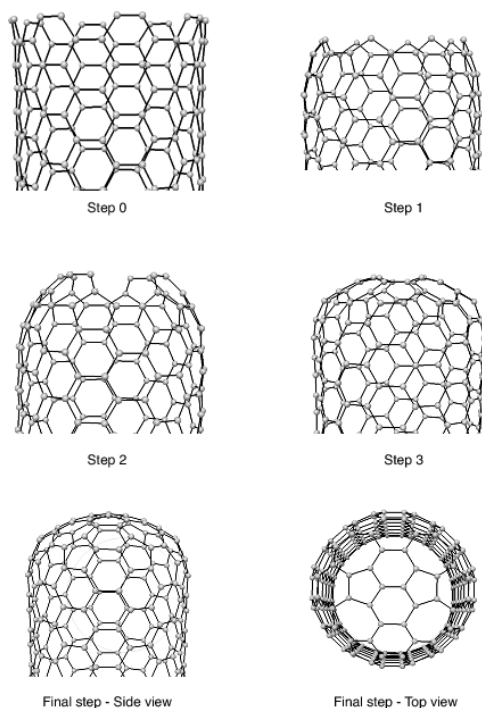
## 4.3. Pharmaceutics and Drug Design

Drug design is the inventive process of finding new medications based on the knowledge of the biological target. The drug is most commonly an organic small molecule which activates or inhibits the function of a biomolecule such as a protein, which in turn results in a therapeutic benefit to the patient. In the most basic sense, drug design involves design of small molecules that are complementary in shape and charge to the biomolecular target to which they interact and therefore will bind to it. Drug design frequently relies on computer modeling techniques. This type of modeling is often referred to as computer-aided drug design.

Structure-based drug design attempts to use the structure of proteins as a basis for designing new ligands by applying accepted principles of molecular recognition. The basic assumption underlying structure-based drug design is that a good ligand molecule should bind tightly to its target. Thus, one of the most important principles for designing or obtaining potential new ligands is to predict the binding affinity of a certain ligand to its target and use it as a criterion for selection.

We develop new methods to estimate the binding affinity using an approximation to the binding free energy. This approximation is assumed to depend on various structural characteristics of a representative set of native complexes with their structure solved to a high resolution. We study and verify different structural characteristics, such as radial distribution functions, and their affect on the binding free energy approximation.

## 4.4. Nano-engineering



*Figure 1. Snapshots of a nanotube capping process with the adaptive interactive modeler. Thanks to the adaptive methodology, this operation can be done in a few minutes.*

In general, we want to develop methods to ease nano-engineering of artificial nanosystems, such as the ones described above (DNA nanotechnology, nano-mechanisms, etc.). We have shown, for example, that our incremental and adaptive algorithms allow us to easily edit and model complex shapes, such as a nanotube (Fig. 1) and the “nano-pillow” below (Fig. 2). Please read more about the SAMSON software platform for more examples.

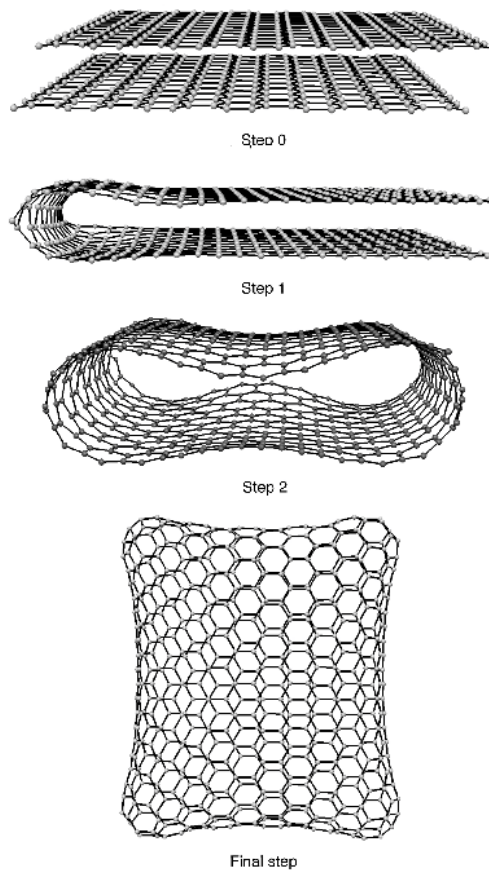


Figure 2. Different steps to prototype a “nano-pillow” with the adaptive interactive modeler.

## **POEMS Project-Team**

### **4. Application Domains**

#### **4.1. Acoustics**

Two particular subjects have retained our attention recently.

Aeroacoustics, or more precisely, acoustic propagation in a moving compressible fluid, has been for our team a very challenging topic, which gave rise to a lot of open questions, from the modeling until the numerical approximation of existing models. Our works in this area are partially supported by Airbus Group. The final objective is to reduce the noise radiated by planes.

Musical acoustics constitutes a particularly attractive application. We are concerned by the simulation of musical instruments. The objective is both a better understanding of the behavior of existing instruments and an aid for the manufacturing of new instruments. We have successively considered the timpani, the guitar and the piano. This activity is continuing in the framework of the European Project BATWOMAN.

#### **4.2. Electromagnetism**

Applied mathematics for electromagnetism during the last ten years have mainly concerned stealth technology and electromagnetic compatibility. These areas are still motivating research in computational sciences (large scale computation) and mathematical modeling (derivation of simplified models for multiscale problems). These topics are developed in collaboration with CEA, DGA and ONERA.

Electromagnetic propagation in non classical media opens a wide and unexplored field of research in applied mathematics. This is the case of wave propagation in photonic crystals, metamaterials or magnetized plasmas. Two ANR projects (METAMATH and CHROME) support this research.

Other subjects are motivated by our partnership with CEA-LIST concerning the simulation of non-destructive testing methods: the development of asymptotic models for complex electromagnetic networks and the simulation by integral equations of eddy current phenomena.

#### **4.3. Elastodynamics**

Wave propagation in solids is with no doubt, among the three fundamental domains that are acoustics, electromagnetism and elastodynamics, the one that poses the most significant difficulties from mathematical and numerical points of view. A major application topic has emerged during the past years : the non destructive testing by ultra-sounds which is the main topic of our collaboration with CEA-LIST. On the other hand, we are developing efficient integral equation modelling for geophysical and civil engineering applications (soil-structure interaction for civil engineering, seismology).

## RAPSODI 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 dioxide sequestration. We refer to [47], [46] 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

The concept for long term storage of high-level radioactive waste in France under study is based on an underground repository. The waste shall be confined in a glass matrix and then placed into cylindrical steel canisters. These containers shall be placed into micro-tunnels in the highly impermeable Callovo-Oxfordian claystone layer at a depth of several hundred meters. At the request of the French nuclear waste management agency ANDRA, investigations are conducted to optimize and finalize this repository concept with the aim to ensure its long-term safety and its reversibility. The long-term safety assessment of the geological repository has to take into account the degradation of the carbon steel used for the waste overpacks and the cell disposal liners, which are in contact with the claystone formation. This degradation is mainly caused by generalized corrosion processes which form a passive layer on the metal surface consisting of a dense oxide inner layer and a porous hydroxide outer layer in contact with the groundwater in the pore space of the claystones. The processes take place under anaerobic conditions, since the groundwater is anoxic.

As a tool to investigate the corrosion processes at the surface of the carbon steel canisters, the Diffusion Poisson Coupled Model (DPCM) for corrosion has been developed by Bataillon *et al.* [1]. The numerical approximation of this corrosion model and some associated models by accurate and efficient methods is challenging. Theoretical study of the models (existence of solutions, long time behavior) is also worth of interest.

## 4.3. Complex fluid flow simulations

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

Let us first focus on fluid mixture flows. The fluid is described by its density, its velocity and its pressure. These quantities obey mass and momentum conservation. On the one hand, when we deal with the 2D variable density incompressible Navier-Stokes equations, we aim to study the ability of the numerical scheme to reproduce some instabilities phenomena such as the Rayleigh-Taylor instability. On the other hand, diffuse interface models have gained renewed interest for the last few years in fluid mechanics applications. From a physical viewpoint, they allow to describe some phase transition phenomena. If the Fick's law relates the divergence of the velocity field to derivatives of the density, one obtains the so called Kazhikhov-Smagulov model [61]. Here, the density of the mixture is naturally highly non homogeneous, and the constitutive law accounts for diffusion effects between the constituents of the mixture. The first phenomena that we want to reproduce are the powder-snow avalanches. We investigate the influence of the characteristics parameters (Froude, Schmidt and Reynolds numbers) on the progression of the front. Other similar hydrodynamic models arise in combustion theory or transport of pollutants.

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.

#### 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 the so-called "*a posteriori* error estimators", is consequently necessary to reach a high precision of calculations in order to provide estimations as reliable as possible.

## APICS Project-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 source problems in EEG

**Participants:** Laurent Baratchart, Juliette Leblond, Jean-Paul Marmorat, Christos Papageorgakis, Nicolas Schnitzler.

This work is conducted in collaboration with Maureen Clerc and Théo Papadopoulos from the Athena EPI.

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 [7]. 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 [38][5]. 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.

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 the Athena team at Inria Sophia Antipolis, neuroscience teams in partner-hospitals (la Timone, Marseille), and the BESA company (Munich).

## 4.3. Inverse magnetization problems

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

Generally speaking, inverse potential problems, similar to the one appearing in Section 4.2, 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 Section 8.2.2.

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. This associate team 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 parallel plane at small distance above the slab.

Mathematically speaking, both inverse source problems for EEG from Section 4.2 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 vector potential:

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

outside the volume  $\Omega$  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 [33] and Section 6.1.2, but the two situations share a substantial Mathematical common core.

#### 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.

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.



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.

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 filter is 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 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 the response being respectively close to 0 and 1 outside the interval measurement, cf. Section 3.3.1). This provides us with a scattering matrix of order roughly 1/4 of the number of data points.
- Approximating this scattering matrix by a rational transfer-function of fixed degree (8 in this example) via the Endymion or RARL2 software (cf. Section 3.3.2.2).
- A realization of the transfer function is thus obtained, and some additional symmetry constraints are 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).

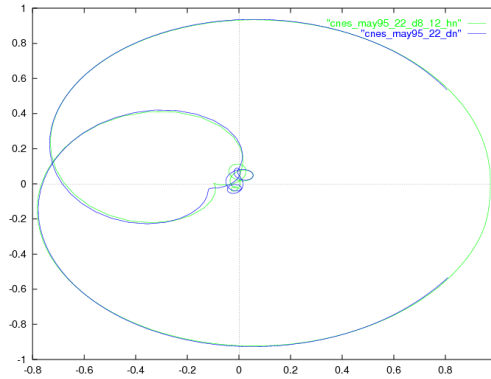


Figure 2. Nyquist Diagram. Rational approximation (degree 8) and data -  $S_{22}$ .

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 also 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 [8]. 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 can be chosen freely. The denominator  $q$  is obtained as the unique stable unitary polynomial solving the classical Feldtkeller spectral equation:

$$qq^* = p_1p_1^* + p_2p_2^*.$$

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 power dividers or when considering the synthesis of filters under matching conditions. The efficient derivation of multiplexers responses is among the team's recent investigation, where techniques based on constrained Nevanlinna-Pick interpolation problems are being considered (see Section 6.2).

Through contacts with CNES (Toulouse) and UPV (Bilbao), Apics got further 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 [75]. This has had tremendous impact on design, and there is a growing demand for software analyzers.

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 7.2 .

## BIPOP Project-Team

# 4. Application Domains

## 4.1. Computational neuroscience

Modeling in neuroscience makes extensive use of nonlinear dynamical systems with a huge number of interconnected elements. Our current theoretical understanding of the properties of neural systems is mainly based on numerical simulations, from single cell models to neural networks. To handle correctly the discontinuous nature of integrate-and-fire networks, specific numerical schemes have to be developed. Our current works focus on event-driven, time-stepping and voltage-stepping strategies, to simulate accurately and efficiently neuronal networks. Our activity also includes a mathematical analysis of the dynamical properties of neural systems. One of our aims is to understand neural computation and to develop it as a new type of information science [19], [20].

## 4.2. Electronic circuits

Whether they are integrated on a single substrate or as a set of components on a board, electronic circuits are very often a complex assembly of many basic components with non linear characteristics. The IC technologies now allow the integration of hundreds of millions of transistors switching at GHz frequencies on a die of  $1\text{cm}^2$ . It is out of the question to simulate a complete IC with standard tools such as the SPICE simulator. We currently work on a dedicated plug-in able to simulate a whole circuit comprising various components, some modelled in a nonsmooth way [1].

## 4.3. Walking robots

As compared to rolling robots, the walking ones – for example hexapods – possess definite advantages whenever the ground is not flat or free: clearing obstacles is easier, holding on the ground is lighter, adaptivity is improved. However, if the working environment of the system is adapted to man, the biped technology must be preferred, to preserve good displacement abilities without modifying the environment. This explains the interest displayed by the international community in robotics toward humanoid systems, whose aim is to back man in some of his activities, professional or others. For example, a certain form of help at home to disabled persons could be done by biped robots, as they are able to move without any special adaptation of the environment.

## 4.4. Computer graphics animation

Computer graphics animation is dedicated to the numerical modeling and simulation of physical phenomena featuring a high visual impact. Typically, deformable objects prone to strong deformation, large displacements, complex and nonlinear or even nonsmooth behavior, are of interest for this community. We are interested in two main mechanical phenomena: on the one hand, the behavior of slender (nonlinear) structures such as rods, plates and shells; on the other hand, the effect of frictional contact between rigid or deformable bodies. In both cases the goal is to design realistic, efficient, robust, and controllable computational models. Whereas the problem of collision detection has become a mature field those recent years, simulating the collision response (in particular frictional contacts) in a realistic, robust and efficient way, still remains an important challenge. Another related issue we began to study is the simulation of heterogeneous objects such as granular or fibrous materials, which requires the design of new high-scales models for dynamics and contacts; indeed, for such large systems, simulating each interacting particle/fiber individually would be too much time-consuming for typical graphics applications. We also pursue some study on the design of high-order models for slender structures such as rods, plates or shells. Our current activity includes the static inversion of mechanical objects, which is of great importance in the field of artistic design, for the making of movies

and video games for example. Such problems typically involve geometric fitting and parameters identification issues, both resolved with the help of constrained optimization. Finally, we are interested in studying certain discrepancies (inexistence of solution) due to the combination of incompatible models such as contacting rigid bodies subject to Coulomb friction.

## **4.5. Multibody Systems: Modeling, Control, Waves, Simulation**

Multibody systems are assemblies of rigid or flexible bodies, typically modeled with Newton-Euler or Lagrange dynamics, with bilateral and unilateral constraints, with or without tangential effects like friction. These systems are highly nonlinear and nonsmooth, and are therefore challenging for modeling aspects (impact dynamics, especially multiple –simultaneous– collisions), feedback control [10], state observation, as well as numerical analysis and simulation (software development) [2], [4], [5]. Biped robots are a particular, interesting subclass of multibody systems subject to various constraints. Granular materials are another important field, in which nonlinear waves transmissions are crucial (one celebrated example being Newton's cradle) [18], [13], [6], [14]. Fibers assemblies [11], circuit breakers, systems with clearances, are also studied in the team.

## **4.6. Stability and Feedback Control**

Lyapunov stability of nonsmooth, complementarity dynamical systems is challenging, because of possible state jumps, and varying system's dimension (the system may live on lower-dimensional subspaces), which may induce instability if not incorporated in the analysis [8], [9], [7]. On the other hand, the nonsmoothness (or the set-valuedness) may be introduced through the feedback control, like for instance the well-known sliding-mode controllers or state observers. The time-discretisation of set-valued controllers is in turn of big interest [3]. The techniques we study originate from numerical analysis in Contact Mechanics (the Moreau-Jean time-stepping algorithm) and are shown to be very efficient for chattering suppression and Lyapunov finite-time stability.

## **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.

#### **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.

#### **4.3. Energy production planning**

We work with colleagues from U. Chile, in the framework of Inria Chile, on the management of electricity production and storage for a microgrid.

## **DISCO Project-Team**

### **4. Application Domains**

#### **4.1. Control of engineering systems**

The team considers control problems in the aeronautic area and studies delay effects in automatic visual tracking on mobile carriers in collaboration with SAGEM.

#### **4.2. Analysis and Control of life sciences systems**

The team is also 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.

#### **4.3. Energy Management**

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



## GECO Project-Team

# 4. Application Domains

## 4.1. Quantum control

The issue of designing efficient transfers between different atomic or molecular levels is crucial in atomic and molecular physics, in particular because of its importance in those fields such as photochemistry (control by laser pulses of chemical reactions), nuclear magnetic resonance (NMR, control by a magnetic field of spin dynamics) and, on a more distant time horizon, the strategic domain of quantum computing. This last application explicitly relies on the design of quantum gates, each of them being, in essence, an open loop control law devoted to a prescribed simultaneous control action. NMR is one of the most promising techniques for the implementation of a quantum computer.

Physically, the control action is realized by exciting the quantum system by means of one or several external fields, being them magnetic or electric fields. The resulting control problem has attracted increasing attention, especially among quantum physicists and chemists (see, for instance, [89], [94]). The rapid evolution of the domain is driven by a multitude of experiments getting more and more precise and complex (see the recent review [50]). Control strategies have been proposed and implemented, both on numerical simulations and on physical systems, but there is still a large gap to fill before getting a complete picture of the control properties of quantum systems. Control techniques should necessarily be innovative, in order to take into account the physical peculiarities of the model and the specific experimental constraints.

The area where the picture got clearer is given by finite dimensional linear closed models.

- **Finite dimensional** refers to the dimension of the space of wave functions, and, accordingly, to the finite number of energy levels.
- **Linear** means that the evolution of the system for a fixed (constant in time) value of the control is determined by a linear vector field.
- **Closed** refers to the fact that the systems are assumed to be totally disconnected from the environment, resulting in the conservation of the norm of the wave function.

The resulting model is well suited for describing spin systems and also arises naturally when infinite dimensional quantum systems of the type discussed below are replaced by their finite dimensional Galerkin approximations. Without seeking exhaustiveness, let us mention some of the issues that have been tackled for finite dimensional linear closed quantum systems:

- controllability [32],
- bounds on the controllability time [28],
- STIRAP processes [99],
- simultaneous control [72],
- optimal control ([68], [41], [52]),
- numerical simulations [78].

Several of these results use suitable transformations or approximations (for instance the so-called rotating wave) to reformulate the finite-dimensional Schrödinger equation as a sub-Riemannian system. Open systems have also been the object of an intensive research activity (see, for instance, [33], [69], [90], [47]).

In the case where the state space is infinite dimensional, some optimal control results are known (see, for instance, [37], [48], [65], [38]). The controllability issue is less understood than in the finite dimensional setting, but several advances should be mentioned. First of all, it is known that one cannot expect exact controllability on the whole Hilbert sphere [98]. Moreover, it has been shown that a relevant model, the quantum oscillator, is not even approximately controllable [91], [81]. These negative results have been more recently completed by positive ones. In [39], [40] Beauchard and Coron obtained the first positive controllability result for a quantum particle in a 1D potential well. The result is highly nontrivial and is based on Coron's return method (see [54]). Exact controllability is proven to hold among regular enough wave functions. In particular, exact controllability among eigenfunctions of the uncontrolled Schrödinger operator can be achieved. Other important approximate controllability results have then been proved using Lyapunov methods [80], [85], [66]. While [80] studies a controlled Schrödinger equation in  $\mathbb{R}$  for which the uncontrolled Schrödinger operator has mixed spectrum, [85], [66] deal mainly with general discrete-spectrum Schrödinger operators.

In all the positive results recalled in the previous paragraph, the quantum system is steered by a single external field. Different techniques can be applied in the case of two or more external fields, leading to additional controllability results [57], [44].

The picture is even less clear for nonlinear models, such as Gross–Pitaevski and Hartree–Fock equations. The obstructions to exact controllability, similar to the ones mentioned in the linear case, have been discussed in [63]. Optimal control approaches have also been considered [36], [49]. A comprehensive controllability analysis of such models is probably a long way away.

## 4.2. Neurophysiology

At the interface between neurosciences, mathematics, automatics and humanoid robotics, an entire new approach to neurophysiology is emerging. It arouses a strong interest in the four communities and its development requires a joint effort and the sharing of complementary tools.

A family of extremely interesting problems concerns the understanding of the mechanisms supervising some sensorial reactions or biomechanics actions such as image reconstruction by the primary visual cortex, eyes movement and body motion.

In order to study these phenomena, a promising approach consists in identifying the motion planning problems undertaken by the brain, through the analysis of the strategies that it applies when challenged by external inputs. The role of control is that of a language allowing to read and model neurological phenomena. The control algorithms would shed new light on the brain's geometric perception (the so-called neurogeometry [87]) and on the functional organization of the motor pathways.

- A challenging problem is that of the understanding of the mechanisms which are responsible for the process of image reconstruction in the primary visual cortex V1.

The visual cortex areas composing V1 are notable for their complex spatial organization and their functional diversity. Understanding and describing their architecture requires sophisticated modeling tools. At the same time, the structure of the natural and artificial images used in visual psychophysics can be fully disclosed only using rather deep geometric concepts. The word "geometry" refers here to the internal geometry of the functional architecture of visual cortex areas (not to the geometry of the Euclidean external space). Differential geometry and analysis both play a fundamental role in the description of the structural characteristics of visual perception.

A model of human perception based on a simplified description of the visual cortex V1, involving geometric objects typical of control theory and sub-Riemannian geometry, has been first proposed by Petitot ([88]) and then modified by Citti and Sarti ([53]). The model is based on experimental observations, and in particular on the fundamental work by Hubel and Wiesel [62] who received the Nobel prize in 1981.

In this model, neurons of V1 are grouped into orientation columns, each of them being sensitive to visual stimuli arriving at a given point of the retina and oriented along a given direction. The retina is modeled by the real plane, while the directions at a given point are modeled by the projective line. The fiber bundle having as base the real plane and as fiber the projective line is called the *bundle of directions of the plane*.

From the neurological point of view, orientation columns are in turn grouped into hypercolumns, each of them sensitive to stimuli arriving at a given point, oriented along any direction. In the same hypercolumn, relative to a point of the plane, we also find neurons that are sensitive to other stimuli properties, such as colors. Therefore, in this model the visual cortex treats an image not as a planar object, but as a set of points in the bundle of directions of the plane. The reconstruction is then realized by minimizing the energy necessary to activate orientation columns among those which are not activated directly by the image. This gives rise to a sub-Riemannian problem on the bundle of directions of the plane.

- Another class of challenging problems concern the functional organization of the motor pathways.

The interest in establishing a model of the motor pathways, at the same time mathematically rigorous and biologically plausible, comes from the possible spillovers in robotics and neurophysiology. It could help to design better control strategies for robots and artificial limbs, yielding smoother and more progressive movements. Another underlying relevant societal goal (clearly beyond our domain of expertise) is to clarify the mechanisms of certain debilitating troubles such as cerebellar disease, chorea and Parkinson's disease.

A key issue in order to establish a model of the motor pathways is to determine the criteria underlying the brain's choices. For instance, for the problem of human locomotion (see [35]), identifying such criteria would be crucial to understand the neural pathways implicated in the generation of locomotion trajectories.

A nowadays widely accepted paradigm is that, among all possible movements, the accomplished ones satisfy suitable optimality criteria (see [97] for a review). One is then led to study an inverse optimal control problem: starting from a database of experimentally recorded movements, identify a cost function such that the corresponding optimal solutions are compatible with the observed behaviors.

Different methods have been taken into account in the literature to tackle this kind of problems, for instance in the linear quadratic case [67] or for Markov processes [86]. However all these methods have been conceived for very specific systems and they are not suitable in the general case. Two approaches are possible to overcome this difficulty. The direct approach consists in choosing a cost function among a class of functions naturally adapted to the dynamics (such as energy functions) and to compare the solutions of the corresponding optimal control problem to the experimental data. In particular one needs to compute, numerically or analytically, the optimal trajectories and to choose suitable criteria (quantitative and qualitative) for the comparison with observed trajectories. The inverse approach consists in deriving the cost function from the qualitative analysis of the data.

### 4.3. Switched systems

Switched systems form a subclass of hybrid systems, which themselves constitute a key growth area in automation and communication technologies with a broad range of applications. Existing and emerging areas include automotive and transportation industry, energy management and factory automation. The notion of hybrid systems provides a framework adapted to the description of the heterogeneous aspects related to the interaction of continuous dynamics (physical system) and discrete/logical components.

The characterizing feature of switched systems is the collective aspect of the dynamics. A typical question is that of stability, in which one wants to determine whether a dynamical system whose evolution is influenced by a time-dependent signal is uniformly stable with respect to all signals in a fixed class ([74]).

The theory of finite-dimensional hybrid and switched systems has been the subject of intensive research in the last decade and a large number of diverse and challenging problems such as stabilizability, observability, optimal control and synchronization have been investigated (see for instance [95], [75]).

The question of stability, in particular, because of its relevance for applications, has spurred a rich literature. Important contributions concern the notion of common Lyapunov function: when there exists a Lyapunov function that decays along all possible modes of the system (that is, for every possible constant value of the signal), then the system is uniformly asymptotically stable. Conversely, if the system is stable uniformly with respect to all signals switching in an arbitrary way, then a common Lyapunov function exists [76]. In the *linear* finite-dimensional case, the existence of a common Lyapunov function is actually equivalent to the global uniform exponential stability of the system [82] and, provided that the admissible modes are finitely many, the Lyapunov function can be taken polyhedral or polynomial [42], [43], [55]. 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 [56] and references therein). Algebraic approaches to prove the stability of switched systems under arbitrary switching, not relying on Lyapunov techniques, have been proposed in [73], [29].

Other interesting issues concerning the stability of switched systems arise when, instead of considering arbitrary switching, one restricts the class of admissible signals, by imposing, for instance, a dwell time constraint [61].

Another rich area of research concerns discrete-time switched systems, where new intriguing phenomena appear, preventing the algebraic characterization of stability even for small dimensions of the state space [70]. It is known that, in this context, stability cannot be tested on periodic signals alone [45].

Finally, let us mention that little is known about infinite-dimensional switched system, with the exception of some results on uniform asymptotic stability ([79], [92], [93]) and some recent papers on optimal control ([60], [100]).

## I4S Project-Team

# 4. Application Domains

## 4.1. Civil Engineering

For at least three decades, monitoring the integrity of the civil infrastructure has been an active research topic because of major economical and societal issues, such as durability and safety of infrastructures, buildings and networks. Control of civil structures began a century ago. At stake is the mastering of the aging of the bridges, as in America (US, Canada) and Great Britain, or the resistance to seismic events and the protection of the cultural heritage, as in Italy and Greece. The research effort in France is very ancient since for example early developments of optical methods to monitor civil structures began in the 70s and SHM practice can be traced back to the 50s with the vibrating wire sensors as strain gauges for dams. Still the number of sensors actually placed on civil structures is kept to a minimum, mainly for cost reasons, but also because the return on investment sensing and data processing technologies is not properly established for civil structures. One of the current thematic priorities of the C2D2 governmental initiative is devoted to construction monitoring and diagnostics. The picture in Asia (Japan, and also China) is somewhat different, in that recent or currently built bridges are equipped with hundreds if not thousands of sensors, in particular the Hong Kong-Shenzen Western Corridor and Stonecutter Bridge projects. However, the actual use of available data for operational purpose remains unclear.

Among the challenges for vibration-based bridges health monitoring, two major issues are the different kinds of (non measured) excitation sources and the environmental effects. Typically the traffic on *and* under the bridge, the wind and also the rain, contribute to excite the structure, and influence the measured dynamics. Moreover, the temperature is also known to affect the eigenfrequencies and mode-shapes, to an extent which can be significant w.r.t. the deviations to be monitored.

Thermomechanical prestress states affect the dynamic and the static behavior of most bridges, not only of very long and flexible ones. So, the reliable and fast determination of the state of prestress and prestrain associated with a temperature field becomes a crucial step in several engineering processes such as the health monitoring of civil structures. The best possible reconstruction of the temperature field could then become part of a complete process including massively distributed sensing of thermomechanical information on the structure, modeling and algorithms for the on-line detection of damages in the sense of abnormalities with regard to a nominal state, the whole chain being encapsulated in professional tools used by engineers in charge of real-life structural monitoring. For lack of an adequate mobilization of the useful multidisciplinary skills, this way remains about unexplored today.

## 4.2. Electrical cable and network monitoring

The fast development of electronic devices in modern engineering systems comes with more and more connections through cables, and consequently, the reliability of electric connections becomes a crucial issue. For example, in a modern automotive vehicle, the total length of onboard cables has tremendously increased during the last decades and is now up to 4km. These wires and connectors are subject to aging or degradation because of severe environmental conditions. In this area, reliability becomes a safety issue. In some other domains, cable defects may have catastrophic consequences. It is thus a crucial challenge to design smart embedded diagnosis systems able to detect wired connection defects in real time. This fact has motivated research projects on methods for fault diagnosis in electric transmission lines and wired networks. Original methods have been recently developed by Inria, notably based on the inverse scattering theory, for cable and network monitoring. Further developments concern both theoretic study and industrial applications.

### **4.3. Aeronautics**

Improved safety and performance and reduced aircraft development and operating costs are major concerns in aeronautics industry. One critical design objective is to clear the aircraft from unstable aero-elastic vibrations (flutter) in all flight conditions. Opening of flight domain requires a careful exploration of the dynamical behavior of the structure subject to vibration and aero-servo-elastic forces. This is achieved via a combination of ground vibration tests and in flight tests. For both types of tests, various sensors data are recorded, and modal analyses are performed. Important challenges of the in-flight modal analyses are the limited choices for measured excitation inputs, and the presence of unmeasured natural excitation inputs (turbulence). Today, structural flight tests require controlled excitation by ailerons or other devices, stationary flight conditions (constant elevation and speed), and no turbulence. As a consequence, flight domain opening requires a lot of test flights and its costly. This is even worse for aircrafts having a large number of variants (business jets, military aircrafts). A key challenge is therefore to allow for exploiting more data under more conditions during flight tests: uncontrolled excitation, nonstationary conditions.

## Maxplus Team

### 4. Application Domains

#### 4.1. Systèmes à événements discrets (productique, réseaux)/Discrete event systems (manufacturing systems, networks)

Une partie importante des applications de l'algèbre max-plus provient des systèmes dynamiques à événements discrets [6]. Les systèmes linéaires max-plus, et plus généralement les systèmes dynamiques monotones contractants, fournissent des modèles naturels dont les résultats analytiques peuvent être appliqués aux problèmes d'évaluation de performance. Relèvent de l'approche max-plus, tout au moins sous forme simplifiée : des problèmes de calcul de temps de cycle pour des circuits digitaux [77], des problèmes de calcul de débit pour des ateliers [125], pour des réseaux ferroviaires [76] ou routiers, et l'évaluation de performance des réseaux de communication [67]. L'approche max-plus a été appliquée à l'analyse du comportement temporel de systèmes concurrents, et en particulier à l'analyse de "high level sequence message charts" [71], [135]. Le projet Maxplus collabore avec le projet Metalau, qui étudie particulièrement les applications des modèles max-plus à la modélisation microscopique du trafic routier [142], [139], [105].

##### *English version*

One important part of applications of max-plus algebra comes from discrete event dynamical systems [6]. Max-plus linear systems, and more generally, monotone nonexpansive dynamical systems, provide natural models for which many analytical results can be applied to performance evaluation problems. For instance, problems like computing the cycle time of asynchronous digital circuits [77], or computing the throughput of a workshop [125] or of a transportation network, and performance evaluation problems for communication networks, are often amenable to max-plus algebra, at least in some simplified form, see in particular [76] and [67]. The max-plus approach has been applied to the analysis of the time behaviour of concurrent systems, and in particular, to the analysis of high level sequence message charts [71], [135]. The Maxplus team collaborates with the Metalau team, working particularly on the applications of max-plus models to the microscopic modelling of road traffic [142], [139], [105].

#### 4.2. Commande optimale et jeux/Optimal control and games

La commande optimale et la théorie des jeux ont de nombreuses applications bien répertoriées: économie, finance, gestion de stock, optimisation des réseaux, aide à la décision, etc. En particulier, le projet Mathfi travaille sur les applications à des problèmes de mathématiques financières. Il existe une tradition de collaborations entre les chercheurs des projets Mathfi et Maxplus sur ces questions, voir par exemple [5] qui comprend un résultat exploitant des idées de théorie spectrale non-linéaire, présentées dans [3].

##### *English version*

Optimal control and game theory have numerous well established applications fields: mathematical economy and finance, stock optimization, optimization of networks, decision making, etc. In particular, the Mathfi team works on applications in mathematical finance. There is a tradition of collaboration between researchers of the Maxplus team and of the Mathfi team on these questions, see as an illustration [5] where ideas from the spectral theory of monotone homogeneous maps [3] are applied.

#### 4.3. Recherche opérationnelle/Operations research

L'algèbre max-plus intervient de plusieurs manières en Recherche opérationnelle. Premièrement, il existe des liens profonds entre l'algèbre max-plus et les problèmes d'optimisation discrète, voir [78]. Ces liens conduisent parfois à de nouveaux algorithmes pour les problèmes de recherche opérationnelle classiques,

comme le problème de circuit de poids moyen maximum [85]. Certains problèmes combinatoires, comme des problèmes de programmation disjonctive, peuvent être décomposés par des méthodes de type max-plus [168]. Ensuite, le rôle de l’algèbre max-plus dans les problèmes d’ordonnement est bien connu depuis les années 60, les dates de complétion pouvant souvent être calculées à partir d’équations linéaires max-plus. Plus récemment, des représentations de problèmes d’ordonnement ont pu être obtenues à partir de semi-groupes de matrices max-plus : une première représentation a été obtenue dans [113] pour le cas du “jobshop”, une représentation plus simple a été obtenue dans [136] dans le cas du “flowshop”. Ce point de vue algébrique a été très utile dans le cas du “flowshop” : il permet de retrouver des résultats anciens de dominance et d’obtenir ainsi de nouvelles bornes [136]. Finalement, en regardant l’algèbre max-plus comme une limite de l’algèbre classique, on peut utiliser des outils algébriques en optimisation combinatoire [133].

#### English version

Max-plus algebra arise in several ways in Operations Research. First, there are intimate relations between max-plus algebra and discrete optimisation problems, see [78]. Sometimes, these relations lead to new algorithms for classical Operations Research problems, like the maximal circuit mean [85]. There are also special combinatorial problems, like certain problems of disjunctive programming, which can be decomposed by max-plus type methods [168]. Next, the role of max-plus algebra in scheduling problems has been known since the sixties: completion dates can often be computed by max-plus linear equations. Recently, representations of certain scheduling problems using max-plus matrix semigroups have appeared, a first representation was given in [113] for the jobshop case, a simpler representation was given in [136] in the flowshop case. This algebraic point of view turned out to be particularly fruitful in the flowshop case: it allows one to recover old dominance results and to obtain new bounds [136]. Finally, viewing max-plus algebra as a limit of classical algebra allows to use algebraic tools in combinatorial optimisation [133].

## 4.4. Analyse statique de programmes/Static analysis of computer programs

L’interprétation abstraite est une technique, introduite par P. et R. Cousot [89], qui permet de déterminer des invariants de programmes en calculant des points fixes minimaux d’applications monotones définies sur certains treillis. On associe en effet à chaque point de contrôle du programme un élément du treillis, qui représente une sur-approximation valide de l’ensemble des valeurs pouvant être prises par les variables du programme en ce point. Le treillis le plus simple exprimant des propriétés numériques est celui des produits Cartésiens d’intervalles. Des treillis plus riches permettent de mieux tenir compte de relations entre variables, en particulier, des classes particulières de polyèdres sont souvent employées.

Voici, en guise d’illustration, un petit exemple de programme, avec le système de point fixe associé, pour le treillis des intervalles:

```
void main() {
  int x=0;      // 1
  while (x<100) { // 2
    x=x+1;     // 3
  }           // 4
}
```

$$\begin{aligned}
 x_1 &= [0, 0] \\
 x_2 &= ] - \infty, 99] \cap (x_1 \cup x_3) \\
 x_3 &= x_2 + [1, 1] \\
 x_4 &= [100, +\infty[ \cap (x_1 \cup x_3)
 \end{aligned}$$

Si l’on s’intéresse par exemple aux valeurs maximales prise par la variable  $x$  au point de contrôle 2, soit  $x_2^\dagger := \max x_2$ , après une élimination, on parvient au problème de point fixe:

$$x_2^\dagger = \min(99, \max(0, x_2^\dagger + 1)) , \quad (3)$$

qui a pour plus petite solution  $x_2^\dagger = 99$ , ce qui prouve que  $x$  est majoré par 99 au point 2.



On reconnaît ici un opérateur de point fixe associé à un problème de jeux à deux joueurs et somme nulle. Cette analogie est en fait générale, dans le cadre d’une collaboration que l’équipe entretient depuis plusieurs années avec l’équipe MeASI d’Eric Goubault (CEA et LIX), spécialiste d’analyse statique, nous avons en effet mis progressivement en évidence une correspondance [88], [110], entre les problèmes de jeux à somme nulle et les problèmes d’analyse statique, qui peut se résumer par le dictionnaire suivant:

|                                    |   |
|------------------------------------|---|
| Jeux                               | Interprétation abstraite  |
| système dynamique                  | programme   |
| opérateur de Shapley               | fonctionnelle   |
| espace d’état                      | (# points de contrôle) $\times$ (# degrés de liberté du treillis) |
| problème en horizon $n$            | exécution de $n$ pas  |
| limite du problème en horizon fini | invariant optimal (borne)   |
| itération sur les valeurs          | itération de Kleene   |

Pour que le nombre d’états du jeu soit fini, il est nécessaire de se limiter à des treillis d’ensembles ayant un nombre fini de degrés de liberté, ce qui est le cas de domaines communément utilisés (intervalles, ensembles définis par des contraintes de potentiel de type  $x_i - x_j \leq c$ , mais aussi, les “templates” qui sont des sous-classes de polyèdres introduits récemment par Sankaranarayanan, Sipma et Manna [160]). L’ensemble des actions est alors fini si on se limite à une arithmétique affine. Signalons cependant qu’en toute généralité, on aboutit à des jeux avec un taux d’escompte négatif, ce qui pose des difficultés inédites. Cette correspondance entre jeux et analyse statique est non intuitive, au sens où les actions du minimiseur consistent à sélectionner des points extrêmes de certains polyèdres obtenus par un mécanisme de dualité.

Une pathologie bien répertoriée en analyse statique est la lenteur des algorithmes de point fixe, qui peuvent effectuer un nombre d’itérations considérable (99 itérations pour obtenir le plus petit point fixe de (8)). Celle-ci est usuellement traitée par des méthodes d’accélération de convergence dites d’élargissement et rétrécissement [90], qui ont cependant l’inconvénient de conduire à une perte de précision des invariants obtenus. Nous avons exploité la correspondance entre analyse statique et jeux pour développer des algorithmes d’une nature très différente, s’inspirant de nos travaux antérieurs sur l’itération sur les politiques pour les jeux répétés [111], [83], [84],[7]. Une version assez générale de cet algorithme, adaptée au domaine des templates, est décrite dans [110] et a fait l’objet d’une implémentation prototype. Chaque itération combine de la programmation linéaire et des algorithmes de graphes. Des résultats expérimentaux ont montré le caractère effectif de la méthode, avec souvent un gain en précision par rapport aux approches classiques, par exemple pour des programmes comprenant des boucles imbriquées.

Ce domaine se trouve être en pleine évolution, un enjeu actuel étant de traiter d’une manière qui passe à l’échelle des invariants plus précis, y compris dans des situations où l’arithmétique n’est plus affine.

#### *English version*

The abstract interpretation method introduced by P. and R. Cousot [89], allows one to determine automatically invariants of programs by computing the minimal fixed point of an order preserving map defined on a complete lattice. To every breakpoint of the program is associated an element of the lattice, which yields a valid overapproximation of the set of reachable values of the vectors of variables of the program, at this breakpoint. The simplest lattice expressing numerical invariants consists of Cartesian products of intervals. More sophisticated lattices, taking into account relations between variables, consisting in particular of subclasses of polyhedra, are often used.

As an illustration, we gave before Eqn (8) a simple example of program, together with the associated fixed-point equation. In this example, the value of the variable  $x$  at the breakpoint 2 is bounded by the smallest solution  $x_2^+$  of the fixed point problem (8), which is equal to 99.

The fixed point equation (8) is similar to the one arising in the theory of zero-sum repeated games. This analogy turns out to be general. Un a series of joint works of our team with the MeASI team of Eric Goubault (CEA and LIX), we brought progressively to light a correspondence [88], [110], between the zero-sum game problems and the static analysis problems, which can be summarized by the following dictionary:

|                                   |   |
|-----------------------------------|---|
| Games                             | Abstract interpretation                         |
| dynamical system                  | program   |
| Shapley operator                  | functional                                      |
| state space                       | (# breakpoints) $\times$ (# degrees of freedom) |
| horizon $n$ problem               | execution of $n$ logical steps                  |
| limit of the value in horizon $n$ | optimal invariant (bound)                       |
| value iteration                   | Kleene iteration                                |

For the game to have a finite state space, we must restrict our attention to lattices of sets with a finite number of degrees of freedom, which is the case of the domains commonly used in static analysis (intervals, sets defined by potentials constraints of the form  $x_i - x_j \leq \text{cst}$ , and also the subclasses of polyhedra called “templates”, introduced recently by Sankaranarayanan, Sipma and Manna [160]). Then, the action space is finite if the arithmetics of the program is affine. However, in full generality, the games we end up with have a negative discount rate, which raises difficulties which are unfamiliar from the game theory point of view. This correspondence between games and static analysis turns out to be non intuitive, in that the action of the minimizer consist of selecting an extreme point of a polyhedron arising from a certain duality construction.

A well known pathology in static analysis is the fact that the standard Kleene fixed point algorithm may have a very slow behavior (99 iterations are needed to get the smallest fixed point of (8)). This is usually solved by using some accelerations of convergence, called widening and narrowing [90], which however lead to a loss of precision. We exploited the correspondence between static analysis and games to develop algorithms of a very different nature, inspired by our earlier work on policy iteration for games [111], [83], [84],[7]. A rather general version of this policy iteration algorithm, adapted to the domain of templates, is described in [110], together with a prototype implementation. Every iteration combines linear programming and combinatorial algorithms. Some experimental results indicate that the method often leads to invariants which are more accurate than the ones obtained by alternative methods, in particular for some programs with nested loops.

This topic of research is currently evolving, a question of current interest being to find accurate invariants, in a scalable way, in situations in which the arithmetics is not affine.

## 4.5. Autres applications/Other applications

L’algèbre max-plus apparaît de manière naturelle dans le calcul de scores de similitudes dans la comparaison de séquences génétiques. Voir par exemple [87].

### *English version*

Max-plus algebra arises naturally in the computation of similarity scores, in biological sequence comparison. See for instance [87].

## MCTAO Project-Team

### 4. Application Domains

#### 4.1. Space engineering, satellites, low thrust control

Space engineering is very demanding in terms of safe and high-performance control laws (for instance optimal in terms of fuel consumption, because only a finite amount of fuel is onboard a satellite for all its “life”). It is therefore prone to real industrial collaborations.

We are especially interested in trajectory control of space vehicles using their own propulsion devices, outside the atmosphere. Here we discuss “non-local” control problems (in the sense of section 3.1 point 1): orbit transfer rather than station keeping; also we do not discuss attitude control.

In the geocentric case, a space vehicle is subject to

- gravitational forces, from one or more central bodies (the corresponding acceleration is denoted by  $F_{\text{grav}}$  below),
- a thrust, the control, produced by a propelling device; it is the  $G u$  term below; assume for simplicity that control in all directions is allowed, *i.e.*  $G$  is an invertible matrix
- other “perturbating” forces (the corresponding acceleration is denoted by  $F_2$  below).

In position-velocity coordinates, its dynamics can be written as

$$\ddot{x} = F_{\text{grav.}}(x, t) \left[ + F_2(x, \dot{x}, t) \right] + G(x, \dot{x}) u, \quad \|u\| \leq u_{\text{max}}. \quad (4)$$

In the case of a single attracting central body (the earth) and in a geocentric frame,  $F_{\text{grav.}}$  does not depend on time, or consists of a main term that does not depend on time and smaller terms reflecting the action of the moon or the sun, that depend on time. The second term is often neglected in the design of the control at first sight; it contains terms like atmospheric drag or solar pressure.  $G$  could also bear an explicit dependence on time (here we omit the variation of the mass, that decreases proportionally to  $\|u\|$ ).

##### 4.1.1. Low thrust

Low thrust means that  $u_{\text{max}}$  is small, or more precisely that the maximum magnitude of  $G u$  is small with respect to the one of  $F_{\text{grav.}}$  (but in general not compared to  $F_2$ ). Hence the influence of the control is very weak instantaneously, and trajectories can only be significantly modified by accumulating the effect of this low thrust on a long time. Obviously this is possible only because the free system is somehow conservative. This was “abstracted” in section 3.5.

*Why low thrust ?* The common principle to all propulsion devices is to eject particles, with some relative speed with respect to the vehicle; conservation of momentum then induces, from the point of view of the vehicle alone, an external force, the “thrust” (and a mass decrease). Ejecting the same mass of particles with a higher relative speed results in a proportionally higher thrust; this relative speed (specific impulse,  $I_{sp}$ ) is a characteristic of the engine; the higher the  $I_{sp}$ , the smaller the mass of particles needed for the same change in the vehicle momentum. Engines with a higher  $I_{sp}$  are highly desirable because, for the same maneuvers, they reduce the mass of “fuel” to be taken on-board the satellite, hence leaving more room (mass) for the payload. “Classical” chemical engines use combustion to eject particles, at a somehow limited speed even with very efficient fuel; the more recent electric engines use a magnetic field to accelerate particles and eject them at a considerably higher speed; however electrical power is limited (solar cells), and only a small amount of particles can be accelerated per unit of time, inducing the limitation on thrust magnitude.

Electric engines theoretically allow many more maneuvers with the same amount of particles, with the drawback that the instant force is very small; sophisticated control design is necessary to circumvent this drawback. High thrust engines allow simpler control procedures because they almost allow instant maneuvers (strategies consist in a few burns at precise instants).

#### 4.1.2. Typical problems

Let us mention two.

- *Orbit transfer or rendez-vous.* It is the classical problem of bringing a satellite to its operating position from the orbit where it is delivered by the launcher; for instance from a GTO orbit to the geostationary orbit at a prescribed longitude (one says rendez-vous when the longitude, or the position on the orbit, is prescribed, and transfer if it is free). In equation (1) for the dynamics,  $F_{\text{grav}}$  is the Newtonian gravitation force of the earth (it then does not depend on time);  $F_2$  contains all the terms coming either from the perturbations to the Newtonian potential or from external forces like radiation pressure, and the control is usually allowed in all directions, or with some restrictions to be made precise.
- *Three body problem.* This is about missions in the solar system leaving the region where the attraction of the earth, or another single body, is preponderant. We are then no longer in the situation of a single central body,  $F_{\text{grav}}$  contains the attraction of different planets and the sun. In regions where two central bodies have an influence, say the earth and the moon, or the sun and a planet, the term  $F_{\text{grav}}$  in (1) is the one of the restricted three body problem and dependence on time reflects the movement of the two “big” attracting bodies.

An issue for future experimental missions in the solar system is interplanetary flight planning with gravitational assistance. Tackling this global problem, that even contains some combinatorial problems (itinerary), goes beyond the methodology developed here, but the above considerations are a brick in this puzzle.

#### 4.1.3. Properties of the control system.

If there are no restrictions on the thrust direction, i.e., in equation (1), if the control  $u$  has dimension 3 with an invertible matrix  $G$ , then the control system is “static feedback linearizable”, and a fortiori flat, see section 3.2. However, implementing the static feedback transformation would consist in using the control to “cancel” the gravitation; this is obviously impossible since the available thrust is very small. As mentioned in section 3.1, point 3, the problem remains fully nonlinear in spite of this “linearizable” structure<sup>0</sup>.

## 4.2. Quantum Control

These applications started by a collaboration between B. Bonnard and D. Sugny (a physicist from ICB) in the ANR project Comoc, localized mainly at the University of Dijon. The problem was the control of the orientation of a molecule using a laser field, with a model that does take into account the dissipation due to the interaction with the environment, molecular collisions for instance. The model is a dissipative generalization of the finite dimensional Schrödinger equation, known as Lindblad equation. It is a 3-dimensional system depending upon 3 parameters, yielding a very complicated optimal control problem that we have solved for prescribed boundary conditions. In particular we have computed the minimum time control and the minimum energy control for the orientation of a two-level system, using geometric optimal control and appropriate numerical methods (shooting and numerical continuation) [32], [31].

<sup>0</sup>However, the linear approximation around any feasible trajectory is controllable (a periodic time-varying linear system); optimal control problems will have no singular or abnormal trajectories.

More recently, based on this project, we have reoriented our control activity towards Nuclear Magnetic Resonance (MNR). In MNR medical imaging, the contrast problem is the one of designing a variation of the magnetic field with respect to time that maximizes the difference, on the resulting image, between two different chemical species; this is the “contrast”. This research is conducted with Prof. S. Glaser (TU-München), whose group is performing both in vivo and in vitro experiments; experiments using our techniques have successfully measured the improvement in contrast between materials chemical species that have an importance in medicine, like oxygenated and de-oxygenated blood, see [30]; this is however still to be investigated and improved. The model is the Bloch equation for spin  $\frac{1}{2}$  particles, that can be interpreted as a sub-case of Lindblad equation for a two-level system; the control problem to solve amounts to driving in minimum time the magnetization vector of the spin to zero (for parameters of the system corresponding to one of the species), and generalizations where such spin  $\frac{1}{2}$  particles are coupled: double spin inversion for instance.

A reference book by B. Bonnard and D. Sugny has been published on the topic [33].

### 4.3. Applications of optimal transport

Optimal Transportation in general has many applications. Image processing, biology, fluid mechanics, mathematical physics, game theory, traffic planning, financial mathematics, economics are among the most popular fields of application of the general theory of optimal transport. Many developments have been made in all these fields recently. Three more specific examples:

- In image processing, since a grey-scale image may be viewed as a measure, optimal transportation has been used because it gives a distance between measures corresponding to the optimal cost of moving densities from one to the other, see e.g. the work of J.-M. Morel and co-workers [54].
- In representation and approximation of geometric shapes, say by point-cloud sampling, it is also interesting to associate a measure, rather than just a geometric locus, to a distribution of points (this gives a small importance to exceptional “outlier” mistaken points); this was developed in Q. Mérigot’s PhD [55] in the GEOMETRICA project-team. The relevant distance between measures is again the one coming from optimal transportation.
- The specific to the type of costs that we have considered in some mathematical work, i.e. these coming from optimal control, are concerned with evolutions of densities under state or velocity constraints. A fluid motion or a crowd movement can be seen as the evolution of a density in a given space. If constraints are given on the directions in which these densities can evolve, we are in the framework of non-holonomic transport problems.

### 4.4. Applications to some domains of mathematics.

Control theory (in particular thinking in terms of inputs and reachable set) has brought novel ideas and progresses to mathematics. For instance, some problems from classical calculus of variations have been revisited in terms of optimal control and Pontryagin’s Maximum Principle [44]; also, closed geodesics for perturbed Riemannian metrics were constructed in [47], [48] using control techniques.

Inside McTAO, a work like [10], [9] is definitely in this line, applying techniques from control to construct some perturbations under constraints of Hamiltonian systems to solve longstanding open questions in the field of dynamical systems.

## 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. Vehicular transportation systems

### 4.2.1. 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: forecasting, so as to provide accurate information to users, e.g., travel times; and 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 prediction, 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/>)

#### 4.2.2. *Advanced and interactive vehicle control*

Car industry has been already identified as a potential homeland application for Networked Control [36], as the evolution of micro-electronics paved the way for introducing distributed control in vehicles. In addition, automotive control systems are becoming the more complex and iterative, as more on-board sensors and actuators are made available through technology innovations. The increasing number of subsystems, coupled with overwhelming information made available through on-board and off-board sensors and communication systems, rises new and interesting challenges to achieve optimal performance while maintaining the safety and the robustness of the total system. Causes of such an increase of complexity/difficulties are diverse: interaction between several control sub-systems (ABS, TCS, ESP, etc.), loss of synchrony between sub-systems, limitations in the computation capabilities of each dedicate processor, etc. The team had several past collaborations with the car industry (Renault since 1992, and Ford).

More recently, in the ANR project VOLHAND (2009-2013), the team has been developing a new generation of electrical power-assisted steering specifically designed for disabled and aged persons.

Currently, on-going work under a grant with IFPEN studies how to save energy and reduce pollution, by controlling a vehicle's speed in a smart urban environment, where infrastructure-to-vehicle and vehicle-to-vehicle communications happen and can be taken into account in the control.

#### 4.3. **Inertial navigation**

Inertial navigation is a research area related to the determination of 3D attitude and position of a rigid body. Attitude estimation is based on data fusion from accelerometers, magnetometers and gyroscopes. Attitude is used in general to determine the linear acceleration, which needs to be integrated after to calculate the position. More recently, in the Persyval project LOCATE-ME (2014-2015), the team has started exploring Pedestrian navigation algorithms in collaboration with the Tyrex team (INRIA-Rhône-Alpes). The goal is to provide guidance to pedestrians, e.g., to first responders after a disaster, or to blind people walking in unfamiliar environments. This tasks is particularly challenging for indoor navigation, where no GPS is available.

#### 4.4. **Multi-robot collaborative coordination**

Due to the cost or the risks of using human operators, many tasks of exploration, or of after-disaster intervention are performed by un-manned drones. When communication becomes difficult, e.g., under water, or in spatial exploration, such robots must be autonomous. Complex tasks, such as exploration, or patrolling, or rescue, cannot be achieved by a single robot, and require a self-coordinated fleet of autonomous devices. NECS team has studied the marine research application, where a fleet of Autonomous Underwater Vehicles (AUVs) self-organize in a formation, adapting to the environment, and reaching a source, e.g., of a pollutant. This has been done in collaboration with IFREMER, within the national project ANR CONNECT and the European FP7 project FeedNetBack [1]. On-going research in the team concerns source localization, with a fleet of mobile robots, including wheeled land vehicles.

#### 4.5. **Control design of hydroelectric powerplants**

We have started a collaboration with ALSTOM HYDRO, on collaborative and reconfigurable resilient control design of hydroelectric power plants. This work is within the framework of the joint laboratory Inria/ALSTOM (see <http://www.inria.fr/innovation/actualites/laboratoire-commun-inria-alstom>). A first concrete collaboration has been established with the CIFRE thesis of Simon Gerwig, who is currently studying how to improve performance of a hydro-electric power-plant outside its design operation conditions, by cancellation of oscillations that occur in such operation range.

**NON-A Project-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<sup>0</sup> 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.

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<sup>0</sup>Here the partiality means that no single quantum measurement is capable of providing the complete information on the state of the system.

## SPHINX Team

# 4. Application Domains

## 4.1. Robotic swimmers

Some companies aim at building biomimetic toys robots that can swim in an aquarium for entertainment purposes (Robotswim)<sup>0</sup> and also for medical objectives. During the last three years, some members of the Inria Project-Team CORIDA<sup>0</sup> (Munnier, Scheid and Takahashi) together with members of the automatics laboratory of Nancy CRAN (Daafouz, Jungers) have initiated an active collaboration (CPER AOC) to construct a swimming ball in a very viscous fluid. This ball has a macroscopic size but since the fluid is highly viscous, its motion is similar to the motion of a nanorobot. Such nanorobots could be used for medical purposes to bring some medicine or perform small surgical operations. In order to get a better understanding of such robotic swimmers, we have obtained control results via shape changes and we have developed simulation tools (see [75], [74], [73]). However, in practice the admissible deformations of the ball are limited since they are realized using piezo-electric actuators. In the next four years, we will take into account these constraints by developing two approaches :

1. Solve the control problem by limiting the set of admissible deformations.
2. Find the “best” location of the actuators, in the sense of being the closest to the exact optimal control.

The main tools for this investigation are the 3D codes that we have developed for simulation of fishes into a viscous incompressible fluid (SUSHI3D) or into a inviscid incompressible fluid (SOLEIL).

## 4.2. Aeronautics

We develop robust and efficient solvers for problems arising in aeronautics (or aerospace) like electromagnetic compatibility and acoustic problems related to noise reduction in an aircraft. Our interest for these issues is motivated by our close contacts with companies like Airbus or “Thales Systèmes Aéroportés”. We develop new software needed by these partners and assist them in integrating these new scientific developments in their home-made solvers. In particular, in collaboration with C. Geuzaine (Université de Liège), we are building a freely available parallel solver based on Domain Decomposition Methods that can handle complex engineering simulations, in terms of geometry, discretization methods as well as physics problems, see <http://onelab.info/wiki/GetDDM>. Part of this development is done through the grant ANR BECASIM (in particular with the postdoc position).

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<sup>0</sup>The website <http://www.robotic-fish.net/> presents a list of several robotic fishes that have been built in the last years.

<sup>0</sup>Most members of SPHINX where members of the former Inria project-team CORIDA

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## DOLPHIN Project-Team

## 4. Application Domains

### 4.1. Transportation and logistics

- **Scheduling problems under uncertainty:** The flow-shop scheduling problem is one of the most well-known problems from scheduling. However, most of the works in the literature use a deterministic single-objective formulation. In general, the minimized objective is the total completion time (makespan). Many other criteria may be used to schedule tasks on different machines: maximum tardiness, total tardiness, mean job flowtime, number of delayed jobs, maximum job flowtime, etc. In the DOLPHIN project, a bi-criteria model, which consists in minimizing the makespan and the total tardiness, is studied. A bi-objective flow-shop problem with uncertainty on the duration, minimizing in addition the maximum tardiness, is also studied. It allows us to develop and test multi-objective (and not only bi-objective) optimization methods under uncertainty.
- **Routing problems under uncertainty:** The vehicle routing problem (VRP) is a well-known problem and it has been studied since the end of the fifties. It has a lot of practical applications in many industrial areas (ex. transportation, logistics, etc). Existing studies of the VRP are almost all concerned with the minimization of the total distance only. The model studied in the DOLPHIN project introduces a second objective, whose purpose is to balance the length of the tours. This new criterion is expressed as the minimization of the difference between the length of the longest tour and the length of the shortest tour. Uncertainty on the demands has also been introduced in the model.

### 4.2. Bioinformatics and Health care

Bioinformatic research is a great challenge for our society and numerous research entities of different specialities (biology, medical or information technology) are collaborating on specific themes.

#### 4.2.1. Genomic and post-genomic studies

Previous studies of the DOLPHIN project mainly deal with genomic and postgenomic applications. These have been realized in collaboration with academic and industrial partners (IBL: Biology Institute of Lille; IPL: Pasteur Institute of Lille; IT-Omics firm).

First, genomic studies aim at analyzing genetic factors which may explain multi-factorial diseases such as diabetes, obesity or cardiovascular diseases. The scientific goal was to formulate hypotheses describing associations that may have any influence on diseases under study.

Secondly, in the context of post-genomic, a very large amount of data are obtained thanks to advanced technologies and have to be analyzed. Hence, one of the goals of the project was to develop analysis methods in order to discover knowledge in data coming from biological experiments.

These problems can be modeled as classical data mining tasks (Association rules, feature selection). As the combinatoric of such problems is very high and the quality criteria not unique, we proposed to model these problems as multi-objective combinatorial optimization problems. Evolutionary approaches have been adopted in order to cope with large scale problems.

Nowadays the technology is still going fast and the amount of data increases rapidly. Within the collaboration with Genes Diffusion, specialized in genetics and animal reproduction for bovine, swine, equine and rabbit species, we study combinations of Single Nucleotide Polymorphisms (SNP) that can explain some phenotypic characteristics. Therefore feature selection for regression is addressed using metaheuristics.

#### **4.2.2. Optimization for health care**

The collaboration with the Alicante company, a major actor in the hospital decision making, deals with knowledge extraction by optimization methods for improving the process of inclusion in clinical trials. Indeed, conducting a clinical trial, allowing for example to measure the effectiveness of a treatment, involves selecting a set of patients likely to participate to this test. Currently existing selection processes are far from optimal, and many potential patients are not considered. The objective of this collaboration consists in helping the practitioner to quickly determine if a patient is interesting for a clinical trial or not. Exploring different data sources (from a hospital information system, patient data...), a set of decision rules have to be generated. For this, approaches from multi-objective combinatorial optimization are implemented, requiring extensive work to model the problem, to define criteria optimization and to design specific optimization methods.

#### **4.2.3. Molecular sampling and docking on large hybrid clusters**

A Phd thesis is started in September 2015 in this context in collaboration with UMONS and University of Strasbourg. Flexible molecular docking is a very complex combinatorial optimization problem especially when two components (ligand and protein) involved in the mechanism are together flexible. To deal in a reasonable time with such highly combinatorial process approximate optimization methods and massively parallel computing are absolutely necessary. The focus of the Ph.D thesis is on the flexibility-aware modeling and the design and implementation of near-approached optimization methods for solving the docking problem on large hybrid clusters including GPU accelerators and MIC coprocessors.

## GEOSTAT Project-Team

# 4. Application Domains

## 4.1. Application Domains

Application aspects in GEOSTAT encompass biomedical data (heartbeat signal analysis with IHU LIRYC, biomedical applications in speech signal analysis) and the study of universe science datasets. GEOSTAT's objectives in analysis of biomedical data hinge on the following observations:

- The analysis and detection of cardiac arrhythmia and pathological voice disorders is a paradigm in nonlinear methodologies applied to these types of signals.
- The classical hypothesis under linear approaches are confronted with strong nonlinearities, aperiodicity and chaotic phenomena present in these signals.
- Existing nonlinear approaches are lacking physiological interpretation. Our objective in this part is to propose new measures based on low-level transition characteristics, these transition phenomena being related to general concepts associated to predictability in complex systems.

## INOCS Team

# 4. Application Domains

## 4.1. Introduction

It is hard to find an aspect of our modern-day economy whose design, management and control do not critically depend on the solution of one or more CS decision problems. Even if they are pervasive, many of them are still not “satisfactorily” solved and constitute a strong challenge to research teams nowadays. The innovative research goals of INOCS have, without doubt, a strategic importance in the application field. CS problems appear in a broad range of application fields such as the next one cited hereafter.

1. *the energy sector* where decisions of distinct nature such as production and distribution are jointly determined;
2. *supply chain management* where location and routing decisions have to be defined jointly even if they refer to different time horizons;
3. *revenue management* where the determination of prices for services or products requires to take explicitly into account the strategic consumers’ behaviour.

## **MISTIS Project-Team**

### **4. Application Domains**

#### **4.1. Image Analysis**

**Participants:** Alexis Arnaud, Aina Frau Pascual, Florence Forbes, Stéphane Girard, Pascal Rubini, Alessandro Chiancone, Thomas Perret, Pablo Mesejo Santiago.

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 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 Laboratoire de Planétologie de Grenoble. We worked on hyperspectral images. In the context of the "pole de competitivite" project I-VP, we worked of images of PC Boards.

#### **4.2. Biology, Environment and Medicine**

**Participants:** Pablo Mesejo Santiago, Aina Frau Pascual, Florence Forbes, Stéphane Girard, Seydou-Nourou Sylla, Marie-José Martinez, Jean-Baptiste Durand.

A second domain of applications concerns biology and medicine. We consider the use of missing data models in epidemiology. We also investigated statistical tools for the analysis of bacterial genomes beyond gene detection. Applications in neurosciences are also considered. Finally, in the context of the ANR VMC project Medup, we studied the uncertainties on the forecasting and climate projection for Mediterranean high-impact weather events.

## **MODAL Project-Team**

### **4. Application Domains**

#### **4.1. Application domains**

Potential application areas of statistical modeling for mixed data are (credit scoring, marketing, environment, medical, economic, hydrology,...), but MODAL favors applications related to biology, phylogeny, genetics and medicine. Members of the team are already experienced in these directions with complementary skills.



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## REALOPT Project-Team

# 4. Application Domains

## 4.1. Introduction

Our group has tackled applications in logistics, transportation and routing [60], [59], [55], [57], in production planning [77] and inventory control [55], [57], in network design and traffic routing [38], [47], [53], [80], [35], [48], [66], [73], in cutting and placement problems [63], [64], [74], [75], [76], [78], and in scheduling [6], [67], [33].

## 4.2. 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 [47]. 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-electronic system installation cost. We developed and compared several decomposition approaches [82], [81], [80] 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 [79]. 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 [53], [54].

We studied several time dependent formulations for the unit demand vehicle routing problem [40], [39]. 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 [72] 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 testes on a set of real-life instances coming from a Russian freight real transportation company. Our algorithmes have been faster on these instances than the current solution approach being used by the company.

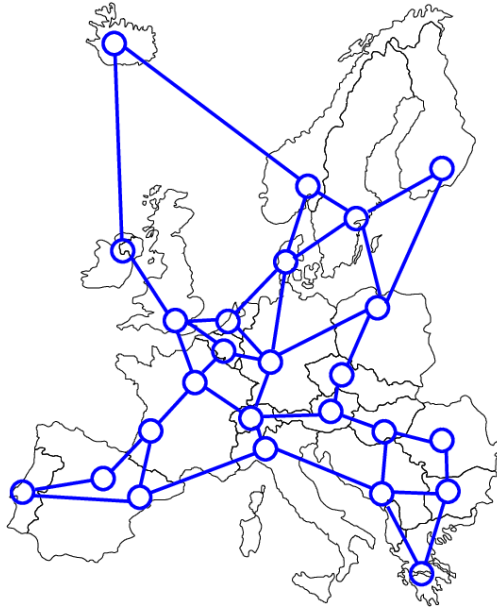


Figure 1. Design of a SDH/SONET european network where demands are multiplexed.

### 4.3. 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 [71]. 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 [31] 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 [57]: we faced a multiple-class integer knapsack problem with setups [56] (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 [50], [49], [52], [51]. 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. 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. They are extra sequencing constraints regarding the production that make the problem even more complex.

Finally, let us add that we are now organizing a european challenge on packing with society Renault: see <http://challenge-esicup-2015.org/>. This challenge is about loading trucks under practical constraints. The final results will be announced in March 2015.

#### 4.4. 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. [58]. 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 [60].

Together with our partner company GAPSO from the associate team SAMBA, we worked on the equipment routing task scheduling problem [65] arising during port operations. In this problem, a set of tasks needs to be performed using equipments of different types with the objective to maximum the weighted sum of performed tasks.

We participated to the project on an airborne radar scheduling. For this problem, we developed fast heuristics [46] and exact algorithms [33]. A substantial research has been done on machine scheduling problems. A new compact MIP formulation was proposed for a large class of these problems [32]. An exact decomposition algorithm was developed for the NP-hard maximizing the weighted number of late jobs problem on a single machine [67]. A dominant class of schedules for malleable parallel jobs was discovered in the NP-hard problem to minimize the total weighted completion time [69]. We proved that a special case of the scheduling problem at cross docking terminals to minimize the storage cost is polynomially solvable [70], [68].

Another application area in which we have successfully developed MIP approaches is in the area of tactical production and supply chain planning. In [30], we proposed a simple heuristic for challenging multi-echelon problems that makes effective use of a standard MIP solver. [29] 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 [34] 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 [42], [41], 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 [36]. We considered train timetabling problems and their re-optimization after a perturbation in the network [44], [43]. 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. 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 [45]. 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 [37].

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## 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 uncertainty in highly complex physical systems.

The other major theme concerns probabilistic modeling in fatigue analysis, in the context of a research collaboration with SAFRAN, a high-technology group (Aerospace propulsion, Aircraft equipment, Defense Security, Communications).

Moreover, a collaboration has begun 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 to be tested on this model selection problem.

## 4.4. Dynamic contrast enhanced imaging

Yves Rozenholc was with SELECT until September 2015, and introduced research for quantifying tumor microcirculation to monitor treatments in cancer. Dynamic Contrast Enhanced (DCE) imaging provides information on the properties of vascular networks. It enables biostatisticians to design biomarkers that can be used for diagnosis, prognosis and treatment monitoring. To make available robust tumoral microcirculation biomarkers in DCE imaging, Yves Rozenholc has developed several tools for denoising and clustering the dynamics found in DCE imaging sequences, and testing equality of survival functions coming from two DCE imaging sequences.

## 4.5. 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.

Yann Vasseur has started a thesis co-supervised by Gilles Celeux and Marie-Laure Martin-Magniette on this topic, which is also an interesting investigation domain for the latent block model developed by SELECT.

SELECT collaborates with Anavaj Sakuntabhai and Benno Schwikowski (Pasteur Institute) on prediction of dengue fever severity from high-dimensional gene expression data. One project involves using/finding new and computationally efficient methods (e.g., 2d isotonic regression, lasso regression) for predicting dengue severity. Due to the high-dimensional nature of the data and low-dimensional nature of the number of individuals, false discovery rate (FDR) methods are used to provide statistical justification of results. A second project involves statistical meta-analysis of newly collected dengue gene expression data along with recently published data sets from other groups.

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.

## 4.6. Pharmacovigilance

A collaboration has been started 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. Valerie Robert has begun a thesis co-supervised by Gilles Celeux and Christine Keribin on this topic, which should enable the development of a new model-based clustering method, inspired by latent block models.

## 4.7. 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 the development of conditional density estimation through GMM, and non-asymptotic model selection, to perform stochastic segmentation of such tensorial datasets. This technique enables the simultaneous accounting for spatial and spectral information, while producing statistically sound information on morphological and physico-chemical aspects of the studied samples.

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## SEQUEL Project-Team

# 4. Application Domains

## 4.1. Recommendation systems in a broad sense

Recommendation systems have been a major field of applications of our research for a few years now. Recommendation systems should be understood in a broad sense, as systems that aim at providing personalized responses/items to users, based on their characteristics, and the environment in which the interaction happens.

In that broad sense, we have collaborated with companies on computational advertizing and recommendation systems. These collaborations have involved research studies on the following issues:

- cold-start problem,
- time varying environment,
- ability to deal with large amounts of users and items,
- ability to design algorithms to respond within a reasonable amount of time, usually below 1 millisecond.

We have also competed in challenges, winning some of them <sup>0</sup>, and we have also organized a challenge <sup>0</sup>, on those topics.

A company has been awarded an innovation award in 2015, thanks to the research work done in collaboration with SEQUEL (*cf. sec. 1*).

In these works, we develop an original <sup>0</sup> point of view on such systems. While traditional (before say 2010) recommendation systems were seen as solving a supervised learning task, or a ranking task, we have developed the idea that recommender systems are really a problem of sequential decision making under uncertainty.

We also started a new work aiming to introduce deep learning in recommender systems. An engineer (Florian Strub) was recruited to work on this topic and presented some results at the NIPS'2015 workshop on "Machine Learning for (e-)Commerce". Moreover we released some code to handle sparse data with the Torch7 framework and GPUs <https://github.com/fstrub95/nnsparse>.

## 4.2. Spoken dialog systems

A Spoken Dialogue System (SDS) is a system enabling human people to interact with machines through speech. In contrast with command-and-control systems or question-answering systems that react to a single utterances, SDS build a real interaction over time and try to achieve complex tasks (like hotel booking, appointment scheduling etc.) by gathering pieces of information through several turns of dialogue. To do so, besides the required speech and language processing modules (*e.g.* speech recognition and synthesis, language understanding and generation), there is a need for a dialogue management module that decides what to say in any situation so as to achieve the goal in the most natural and efficient way, recovering from speech processing errors in a seamless manner.

The dialogue management module is thus taking sequences of decisions to achieve a long-term goal in an unknown, noisy and hard to model environment (since it includes human users). For this reason, we work on machine learning techniques such as reinforcement and imitation learning to optimize this specific sequential decision making under uncertainty problem.

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<sup>0</sup>SEQUEL ranked first and second at the "Pascal Exploration & Exploitation Challenge 2011"; SEQUEL ranked first at the "RecSys Challenge 2014: User Engagement as Evaluation".

<sup>0</sup>ICML 2012 new Challenges for Exploration & Exploitation 3.

<sup>0</sup>the originality fades away as years pass since this idea is exploited by other researchers.

In addition to bring novel and efficient solutions to this problem, we are interested in the new challenges brought to our research in machine learning by this type of application. Indeed, having the human in the learning loop typically requires dealing with non-stationarity, data-efficiency, safety as well as cooperation and imitation.

We collaborate with companies such as Orange Labs on this topic and several projects are ongoing (ANR MaRDi, CHIST-ERA IGLU). We will also be participating to a H2020 project on human robot-interaction starting in 2016 (BabyRobot). We organised a workshop at ICML this year: Machine Learning for Interactive Systems (MLIS). Olivier Pietquin was invited as a panelist at the NIPS Workshop on spoken language understanding and dialogue.

### **4.3. Adaptive/learning systems more generally**

Reinforcement learning leads to the design of systems that adapts their behavior to their environment, hence adaptive systems. We have worked on various applications of this idea, beyond the two main applications domaines mentioned above (recommendation systems, and spoken dialog systems). Let us briefly mention: educative tutoring systems; adaptive heating system in buildings; players that adapt their strength to that of their human opponent; bioreactor.

### **4.4. Prediction in general**

Since the goal of our research is to design systems that learn to act in an optimal way in their environment, prediction is a major issue. Hence, we are doing some research activities on this particular task, without always being in direct connection with learning a policy.

We have done some research in the area of prediction web-server load in a non stationary environment. We also have activities in the prediction in bug in software code.



## **SIERRA Project-Team**

# **4. Application Domains**

## **4.1. Application Domains**

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. In collaboration with Telecom Paris-tech.
- Neuro-imaging: brain-computer interface (fMRI, EEG, MEG). In collaboration with the Parietal project-team.

## TAO Project-Team

# 4. Application Domains

## 4.1. Energy Management

Energy management, our priority application field, involves sequential decision making with:

- stochastic uncertainties (typically weather);
- both high scale combinatorial problems (as induced by nuclear power plants) and non-linear effects;
- high dimension (including hundreds of hydroelectric stocks);
- multiple time scales:
  - minutes (dispatching, ensuring the stability of the grid), essentially beyond the scope of our work, but introducing constraints for our time scales;
  - days (unit commitment, taking care of compromises between various power plants);
  - years, for evaluating marginal costs of long term stocks (typically hydroelectric stocks);
  - decades, for investments.

Significant challenges also include:

- spatial distribution of problems; due to capacity limits we can not consider a power grid like Europe + North Africa as a single “production = demand” constraint; with extra connections we can equilibrate excess production by renewables for remote areas, but not in an unlimited manner.
- other uncertainties, which might be modeled by adversarial or stochastic frameworks (e.g. technological breakthroughs, decisions about ecological penalization).

We have had several related projects (Citines, a European (FP7) project; IOMCA, a ANR project), and we now work on the POST project, a ADEME BIA about investments in power systems. Our collaboration with company Artelys (working on optimization in general, and in particular on energy management) is formalized as an Inria ILAB.

**Technical challenges:** Our work focuses on the combination of reinforcement learning tools, with their anytime behavior and asymptotic guarantees, with existing fast approximate algorithms. Our goal is to extend the state of the art by taking into account non-linearities which are often neglected in power systems due to the huge computational cost. We study various modelling errors, such as bias due to finite samples, linearization, and propose corrections.

**Related Activities:**

- Joint team with Taiwan, namely the Indema associate team (see Section 9.4.1.1).
- Ilab METIS, in progress with Artelys (see Section 6.6) for industrialization of our work. In particular, the Crystal tool is adopted by the European Community (<http://www.artelys.com/news/120/90/Energy-The-European-Commission-Chooses-Artelys-Crystal>)
- Organization of various forums and meetings around Energy Management
- Visit of Edgar Galvan Lopez also includes applications to energy management, more precisely Demand-Side Management systems. In [40], Differential Evolution is used to generate optimal plans to use the accumulators of electrical vehicles in order to reduce the peak household consumption loads.

## 4.2. TAO & Humanities

Several projects related to research for Humanities and/or research transfer have started in 2015:

- Personal semantics (Gregory Grefenstette). In the current digital world, individuals generate increasing amount of personal data. Our work involves discovering semantic axes for organizing and exploiting this data for personal use.
- Gregorius (Cécile Germain & Gregory Grefenstette). An application of semantic structuring and automatic enrichment of existing digital humanities archives.
- Cartolabe (Ph. Caillou, Gregory Grefenstette, Jean-Daniel Fekete - AVIZ, Michèle Sebag). The Cartolabe project applies machine learning techniques to determine comprehensible structures in unstructured data. The goal is to use raw textual data, and underspecified ontologies, to provide intuitive access to pertinent research activities in a large research organisation.
- AmiQap (Ph. Caillou, Michèle Sebag). The multivariate analysis of questionnaire data relative to the quality of life at work, in relation with the socio-economical indicators of firms, aims at investigating the relationship between quality of life and economic performances (depending on the activity domain).
- Collaborative Hiring (Ph. Caillou, Michèle Sebag). Thomas Schmitt's PhD, started in 2014, aims at handling job offers and demands matching as a collaborative filtering problem.
- IODS (Wikidata for Science).

Significant challenges include some Big Data problems:

- learning interpretable clusters from bottom-up treatment of mixed text and numerical data
- aligning bottom-up clusters with existing manually created top-down structures
- building a unified system integrating the "dire d'experts".

**Partners:**

- AmiQap is funded by ISN, with Telecom SES, RITM and La Fabrique as partners.
- The collaborative hiring study is conducted in cooperation with J.P. Nadal from EHESS.

## ASPI Project-Team

### 4. Application Domains

#### 4.1. Localisation, navigation and tracking

Among the many application domains of particle methods, or interacting Monte Carlo methods, ASPI has decided to focus on applications in localisation (or positioning), navigation and tracking [50], [43], which already covers a very broad spectrum of application domains. The objective here is to estimate the position (and also velocity, attitude, etc.) of a mobile object, from the combination of different sources of information, including

- a prior dynamical model of typical evolutions of the mobile, such as inertial estimates and prior model for inertial errors,
- measurements provided by sensors,
- and possibly a digital map providing some useful feature (terrain altitude, power attenuation, etc.) at each possible position.

In some applications, another useful source of information is provided by

- a map of constrained admissible displacements, for instance in the form of an indoor building map,

which particle methods can easily handle (map-matching). This Bayesian dynamical estimation problem is also called filtering, and its numerical implementation using particle methods, known as particle filtering, has been introduced by the target tracking community [49], [63], which has already contributed to many of the most interesting algorithmic improvements and is still very active, and has found applications in

target tracking, integrated navigation, points and / or objects tracking in video sequences, mobile robotics, wireless communications, ubiquitous computing and ambient intelligence, sensor networks, etc.

ASPI is contributing (or has contributed recently) to several applications of particle filtering in positioning, navigation and tracking, such as geolocalisation and tracking in a wireless network, terrain-aided navigation, and data fusion for indoor localisation.

#### 4.2. Rare event simulation

*See 3.3 , and 5.1 , 5.2 , 5.3 , and 5.4 .*

Another application domain of particle methods, or interacting Monte Carlo methods, that ASPI has decided to focus on is the estimation of the small probability of a rare but critical event, in complex dynamical systems. This is a crucial issue in industrial areas such as

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

In such complex systems, analytical methods cannot be used, and naive Monte Carlo methods are clearly un-efficient to estimate accurately very small probabilities. Besides importance sampling, an alternate widespread technique consists in multilevel splitting [57], where trajectories going towards the critical set are given off-springs, thus increasing the number of trajectories that eventually reach the critical set. This approach not only makes it possible to estimate the probability of the rare event, but also provides realizations of the random trajectory, given that it reaches the critical set, i.e. provides realizations of typical critical trajectories, an important feature that methods based on importance sampling usually miss.

ASPI is contributing (or has contributed recently) to several applications of multilevel splitting for rare event simulation, such as risk assessment in air traffic management, detection in sensor networks, and protection of digital documents.

## **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 which gathers several topics of team is a collaboration started in September 2013 with Airbus Defence & Space. The goal of this project is the optimization of the assembly line of the future European launcher, taking into account several kinds of economical and technical constraints. We have started with a simplified model with five components to be assembled in workshops liable to breakdowns. We have modeled the problem using the Markov Decision Processes (MDP) framework and built a simulator of the process in order to run a simulation-based optimization procedure.

A second example concerns the optimization of the maintenance of a on board system equipped with a HUMS (Health Unit Monitoring Systems) in collaboration with THALES Optronique. 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.

However the spectrum of applications of the topics of the team is larger and may 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. Application Domains**

Risk management, Quantitative finance, Computational Finance, Market Microstructure analysis, Systemic risk, Portfolio optimization, Risk modeling, Option pricing and hedging in incomplete markets, insurance.

## TOSCA Project-Team

# 4. Application Domains

## 4.1. Application Domains

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 practitioners 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 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 from 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 equations is an active area of research since very few results still are available in the literature.