



RESEARCH CENTER

FIELD

**Applied Mathematics, Computation  
and Simulation**

Activity Report 2013

# Section Application Domains

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## **CAD Team**

# **4. Application Domains**

## **4.1. Domain**

Computer Aided Design and Computer Graphics are two Application Domains.

## CALVI Project-Team

# 4. Application Domains

## 4.1. Thermonuclear fusion

Inertial fusion, magnetic fusion, ITER, particle accelerators, laser-matter interaction

Controlled fusion is one of the major prospects for a long term source of energy. Two main research directions are studied: magnetic fusion where the plasma is confined in tokamaks using a large external magnetic field and inertial fusion where the plasma is confined thanks to intense laser or particle beams. The simulation tools we develop can be applied for both approaches.

Controlled fusion is one of the major challenges of the 21st century that can answer the need for a long term source of energy that does not accumulate wastes and is safe. The nuclear fusion reaction is based on the fusion of atoms like Deuterium and Tritium. These can be obtained from the water of the oceans that is widely available and the reaction does not produce long-term radioactive wastes, unlike today's nuclear power plants which are based on nuclear fission.

Two major research approaches are followed towards the objective of fusion based nuclear plants: magnetic fusion and inertial fusion. In order to achieve a sustained fusion reaction, it is necessary to confine sufficiently the plasma for a long enough time. If the confinement density is higher, the confinement time can be shorter but the product needs to be greater than some threshold value.

The idea behind magnetic fusion is to use large toroidal devices called tokamaks in which the plasma can be confined thanks to large applied magnetic field. The international project ITER <sup>1</sup> is based on this idea and aims to build a new tokamak which could demonstrate the feasibility of the concept.

The inertial fusion concept consists in using intense laser beams or particle beams to confine a small target containing the Deuterium and Tritium atoms. The Laser Mégajoule which is being built at CEA in Bordeaux will be used for experiments using this approach.

Nonlinear wave-wave interactions are primary mechanisms by which nonlinear fields evolve in time. Understanding the detailed interactions between nonlinear waves is an area of fundamental physics research in classical field theory, hydrodynamics and statistical physics. A large amplitude coherent wave will tend to couple to the natural modes of the medium it is in and transfer energy to the internal degrees of freedom of that system. This is particularly so in the case of high power lasers which are monochromatic, coherent sources of high intensity radiation. Just as in the other states of matter, a high laser beam in a plasma can give rise to stimulated Raman and Brillouin scattering (respectively SRS and SBS). These are three wave parametric instabilities where two small amplitude daughter waves grow exponentially at the expense of the pump wave, once phase matching conditions between the waves are satisfied and threshold power levels are exceeded. The illumination of the target must be uniform enough to allow symmetric implosion. In addition, parametric instabilities in the underdense coronal plasma must not reflect away or scatter a significant fraction of the incident light (via SRS or SBS), nor should they produce significant levels of hot electrons (via SRS), which can preheat the fuel and make its isentropic compression far less efficient. Understanding how these deleterious parametric processes function, what non uniformities and imperfections can degrade their strength, how they saturate and interdepend, all can benefit the design of new laser and target configuration which would minimize their undesirable features in inertial confinement fusion. Clearly, the physics of parametric instabilities must be well understood in order to rationally avoid their perils in the varied plasma and illumination conditions which will be employed in the National Ignition Facility or LMJ lasers. Despite the thirty-year history of the field, much remains to be investigated.

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<sup>1</sup> <http://www.iter.org>

Our work in modelling and numerical simulation of plasmas and particle beams can be applied to problems like laser-matter interaction, the study of parametric instabilities (Raman, Brillouin), the fast ignitor concept in the laser fusion research as well as for the transport of particle beams in accelerators. Another application is devoted to the development of Vlasov gyrokinetic codes in the framework of the magnetic fusion programme in collaboration with the Department of Research on Controlled Fusion at CEA Cadarache. Finally, we work in collaboration with the American Heavy Ion Fusion Virtual National Laboratory, regrouping teams from laboratories in Berkeley, Livermore and Princeton on the development of simulation tools for the evolution of particle beams in accelerators.

## 4.2. Nanophysics

Kinetic models like the Vlasov equation can also be applied for the study of large nano-particles as approximate models when *ab initio* approaches are too costly.

In order to model and interpret experimental results obtained with large nano-particles, *ab initio* methods cannot be employed as they involve prohibitive computational times. A possible alternative resorts to the use of kinetic methods originally developed both in nuclear and plasma physics, for which the valence electrons are assimilated to an inhomogeneous electron plasma. The LPMIA (Nancy) possesses a long experience on the theoretical and computational methods currently used for the solution of kinetic equation of the Vlasov and Wigner type, particularly in the field of plasma physics.

Using a Vlasov Eulerian code, we have investigated in detail the microscopic electron dynamics in the relevant phase space. Thanks to a numerical scheme recently developed by Filbet et al. [64], the fermionic character of the electron distribution can be preserved at all times. This is a crucial feature that allowed us to obtain numerical results over long times, so that the electron thermalization in confined nano-structures could be studied.

The nano-particle was excited by imparting a small velocity shift to the electron distribution. In the small perturbation regime, we recover the results of linear theory, namely oscillations at the Mie frequency and Landau damping. For larger perturbations nonlinear effects were observed to modify the shape of the electron distribution.

For longer time, electron thermalization is observed: as the oscillations are damped, the center of mass energy is entirely converted into thermal energy (kinetic energy around the Fermi surface). Note that this thermalization process takes place even in the absence of electron-electron collisions, as only the electric mean-field is present.

## **CONCHA Project-Team**

# **4. Application Domains**

## **4.1. Domain 1**



## MICMAC Project-Team

# 4. Application Domains

## 4.1. 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 description of matter, or at least a mesoscopic one, with the equations of continuum mechanics at the macroscopic level.

## 4.2. Computational Statistical Mechanics

The orders of magnitude used in the microscopic description 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  $N_A \sim 10^{23}$ , 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  $1.3 \times 10^{18}$  m<sup>3</sup> of water in the oceans, *i.e.*  $7.2 \times 10^{22}$  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  $N_A$  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  $0.1 \mu\text{s}$ .

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?”

### 4.3. Homogenization and related problems

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

The following observation motivates the idea of coupling atomistic and continuum description 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 after 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, 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 be 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.

## SCIPORT Team

# 4. Application Domains

## 4.1. Automatic Differentiation

Automatic Differentiation of programs gives sensitivities or gradients, that are useful for many types of applications:

- 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. From 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-mode AD is a promising 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 the altitude and speed of the surface.

One particular case of inverse problems is *data assimilation* [31] 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 largely unknown. Only some measures at arbitrary places and times are available. A good initial state is found by solving a least squares problem between the measures 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 [34]. Figure 1 shows an example of a data assimilation exercise using the oceanography code OPA [32] 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 measures 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 grows in complexity, 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. We add random noise to a simulation of the ocean state around the Antarctic, and we remove this noise 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 is sometimes 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 a very efficient approximate solution: 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.

## **SIMPAF Project-Team**

# **4. Application Domains**

## **4.1. Physics**

Our applications to physics concern:

- non-equilibrium statistical physics
- cold atoms
- laser propagation
- Maxwell equations

### ***4.1.1. Non-equilibrium statistical physics***

Describing, understanding, predicting and controlling the complex physical phenomena occurring in classical or quantum dynamical systems with a large or infinite number of degrees of freedom are important issues for equilibrium and non-equilibrium statistical mechanics and remain an important challenge for mathematical physics. Some of the typical questions are the following. How does a collective dynamics emerge from the interactions of individual entities? How to compute transport coefficients in terms of microscopic quantities and more generally, what is the role of the local (microscopic) dynamics on global transport properties? What are the system ergodic properties and how are asymptotic states, if they exist, approached? What are the dynamical mechanisms for approach to equilibrium in such systems?

### ***4.1.2. Cold atoms***

A typical problem we are concerned with is the effect of interactions (modeled by a nonlinearity in the evolution equation) on the localization properties of quantum kicked rotors, experimentally realized in cold-atom experiments.

### ***4.1.3. Laser propagation***

We are interested in variants of the NonLinear Schrödinger Equation (NLSE), which govern the evolution of optical fibers, and in particular photonic crystal fibers (PCF). These are key to information and communication technology, and form an unmatched platform to explore complex nonlinear phenomena.

### ***4.1.4. Maxwell equations***

A posteriori error estimators developed for the Maxwell equations are very useful tools for practical computations. They are implemented in the software "Carmel-3D" (see the softwares section). This numerical code is used in order to study some original applications, like electrical machines or specific actuators. It is also devoted to nondestructive control by the use of Foucault currents, to the simulation of devices using magnetic fluids or of induced currents in human bodies.

## **4.2. Continuum mechanics**

Our applications to continuum mechanics concern:

- the numerical simulation of viscous flows
- the mathematical and numerical derivation of rubber elasticity from polymer physics

### **4.2.1. Numerical simulation of viscous flows**

We are concerned with systems of PDEs describing the evolution of mixture flows. The fluid is described by the density, the velocity and the 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 some instabilities phenomena such as the Raileigh-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 obtain the so called Kazhikhov-Smagulov model. 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. Furthermore, a surface tension force can be added to the momentum equation introducing a specific stress tensor, proposed for the first time by Korteweg. The first phenomena that we try to reproduce are the powder-snow avalanches, but we can also model flows where species (like salt or pollutant) are dissolved in a compressible or incompressible fluid. Other similar hydrodynamic models arise in combustion theory.

Flow control strategies using passive or active devices are crucial tools in order to save energy in transports (especially for cars, trucks or planes), or to avoid the fatigue of some materials arising in a vast amount of applications. Nowadays, shape optimization needs to be completed by other original means, such as porous media located on the profiles, as well as vortex generator jets in order to drive active control.

### **4.2.2. From polymer physics to rubber elasticity**

Our aim is to rigorously derive nonlinear elasticity theory from polymer physics. The starting point is the statistical physics description of polymer-chains. Under some proper rescaling, this discrete model converges to continuum nonlinear elasticity models in the sense of Gamma-convergence. The long-term goal of our approach is to derive practical constitutive laws for rubbers (to be used in nonlinear elasticity softwares) from the discrete model.

## **4.3. Corrosion models**

### **4.3.1. Corrosion modelling of iron based alloy in nuclear waste repository**

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.* [32]. 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 worthy of interest.

### **4.3.2. Corrosion modeling of Ni-base alloys in Pressurized Water Reactor primary water**

The understanding of the oxidation behavior of Ni-base alloys in Pressurized Water Reactor (PWR) primary water is of major importance due to the cations released due to corrosion of the steam generators which is a source of the radioactivity of the primary circuit. Moreover, the oxidation process is the reason of the initiation



of intergranular stress corrosion cracking in some alloys. A numerical model, called EKINOX (Estimation KINetics OXydation), has been developed at CEA [33] in order to simulate the oxide scale growth. This model should be able to calculate the evolutions of concentration profiles of the species and of their point defects in the oxide and in the substrate. Numerical experiments have shown the limits of this existing numerical model, especially the need of very small time steps for the computations ; a macroscopic model has been developed and numerical methods proposed for its simulation.

## BACCHUS Team

# 4. Application Domains

## 4.1. Introduction

We are working on problems that can be written in the following form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_e(\mathbf{U}) - \nabla \cdot \mathbf{F}_v(\mathbf{U}, \nabla \mathbf{U}) = 0 \quad (1)$$

in a domain  $\Omega \subset \mathbb{R}^d$ ,  $d = 1, 2, 3$ , subjected to initial and boundary conditions. The variable  $\mathbf{U}$  is a vector in general, the flux  $\mathbf{F}_e$  is a tensor, as well as  $\mathbf{F}_v$  which also depends on the gradient of  $\mathbf{U}$ . The subsystem

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_e(\mathbf{U}) = 0$$

is assumed to be hyperbolic, the subsystem

$$\frac{\partial \mathbf{U}}{\partial t} - \nabla \cdot \mathbf{F}_v(\mathbf{U}, \nabla \mathbf{U}) = 0$$

is assumed to be elliptic. Last, (1) is supposed to satisfy an entropy inequality. The coefficients or models that define the flux and the boundary conditions can be deterministic or random.

The systems (1) are discretised mesh made of conformal elements. The tessellation is denoted by  $\mathcal{T}_h$ . The simplicies are denoted by  $K_j$ ,  $j = 1, n_e$ , and  $\cup_j K_j = \Omega_h$ , an approximation of  $\Omega$ . The mesh is assumed to be adapted to the boundary conditions. In our methods, we assume a globally continuous approximation of  $\mathbf{U}$  such that  $\mathbf{U}|_{K_j}$  is either a polynomial of degree  $k$  or a more complex approximation such as a Nurbs. For now  $k$  is uniform over the mesh, and let us denote by  $V_h$  the vector space spanned by these functions, taking into account the boundary conditions.

The schemes we are working on have a variational formulation: find  $\mathbf{U} \in V_h$  such that for any  $\mathbf{V} \in V_h$ ,

$$a(\mathbf{U}, \mathbf{V}; \mathbf{U}) = 0.$$

The variational operator  $a(\mathbf{U}, \mathbf{V}; \mathbf{W})$  is a sum of local operator that use only data within elements and boundary elements: it is very local. Boundary conditions can be implemented in a variational formulation or using a penalisation technique, see figure 1. The third argument  $\mathbf{W}$  stands for the way are implemented the non oscillatory properties of the method.

This leads to highly non linear systems to solve, we use typically non linear Krylov space techniques. The cost is reduced thanks to a parallel implementation, the domain is partitionned via Scotch. Mesh balancing, after mesh refinement, is handled via PaMPA. These schemes are implemented in Realfluids and, partially, AeroSol. An example of such a simulation is given by Figure 2.

In case of non deterministic problems, we have a semi-intrusive strategy. The randomness is expressed via  $N$  scalar random parameters (that might be correlated),  $X = (x_1, \dots, x_N)$  with probability measure  $d\mu$  which support is in a subset of  $\mathbb{R}^N$ . The idea of non intrusive methods is to approximate  $d\mu$  either by  $d\mu \approx \sum_j \omega_j \delta_{X_j}$  for  $\omega_j \geq 0$  that sum up to unity, for ‘‘well chosen’’ samples  $X_j$  or by  $d\mu \approx \sum_l \mu(\Omega_l) 1_{X_j} dX$  where the sets  $\Omega_j$  covers the support of  $d\mu$  and are non overlapping.



Figure 1. Adapted mesh for a viscous flow over a triangular wedge.

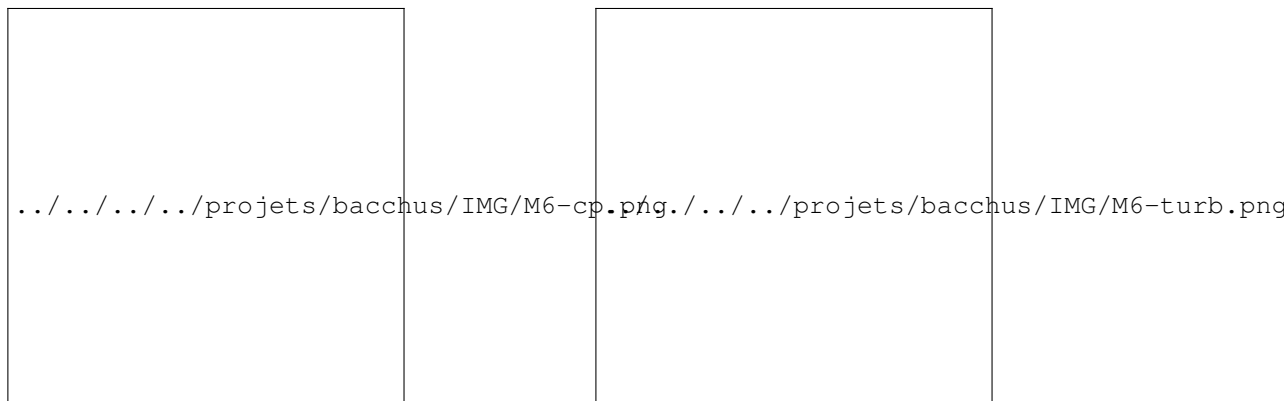


Figure 2. Turbulent flow over a M6 wing (pressure coefficient, mesh by Dassault Aviation).



*Figure 3. Okushiri tsunami experiment. Left : deterministic computation. Right : mean and variance of the wave height in one of the gauges*

Starting from a discrete approximation of (1), we can implement randomness in the scheme. An example is given on figure 3 applied to the shallow water equations with dry shores, when the amplitude of the incoming tsunami wave is not known.

## 4.2. External and internal Aerodynamics

A classical application is the simulation of internal and external flows, with perfect or real gas equation of states, in complex geometries, such as for example the organic dense flows in a turbine cascade. This requires often the use of meshes having heterogeneous structures. We are working with unstructured meshes, either with simplicial elements or mixtures of hex, tets, pyramids and prisms. Mesh refinement can be enable in order to better resolve either the discontinuous flow structures or the capture of boundary layers.

## 4.3. Multiphase flows with mass transfer

Another domain of application is the simulation of multiphase flows. Here, the system (1) need to be supplemented by at least a PDE describing the phase volume changes, and the equation of states of the phases. The system is in most case written in a non-conservative form, so that additional difficulties need to be handled.

Multiphase flows occur in many applications: for petroleum industry, nuclear industry (accident management), engines, pipes, etc.

An adding difficulty is given by the presence of mass transfer between the phases. Cavitation consists in a local pressure drop below the vapor pressure at the liquid temperature, thus creating a phase change and vapor bubbles formation. Their collapse in high-pressure region can dramatically lead to failure, erosion and other undesirable effects. For this reason, there is a strong effort devoted to develop predictive numerical tools for cavitating flows in industrial applications. Unfortunately, an accurate description of interactions between the vapour and liquid phases requires accurate physical models and a way to take into account the dynamics of the interface. Moreover, multiscale effects, turbulence and thermodynamics should be also considered. Cavitation models are typically dependent on two types of parameters: first, on some physical parameters, such as for example the number of bubbles, that is not usually well measured; secondly, on some empiric parameters, useful for fitting and calibration procedures with respect to the experimental data. Therefore, model parameters represent an important source of uncertainty. Moreover, it is not an easy task to well define boundary and initial conditions, because of difficulties encountered in order to control accurately experiments in cavitating flows. As a result, conditions imposed for the setting of a numerical simulation, are affected by a dramatic randomness.

We performed a systematic study for considering the probabilistic properties of the input parameters permitting to capture non-linearities in uncertainty propagation. Moreover, the DEM method has been modified to take into account exotic phenomena with real-gas effects.

## 4.4. Inflight icing and ice shedding

Actual concerns about greenhouse gases lead to changes in aircraft design with an increased use of composite materials. This offers new possibilities for the design of ice protection systems. These systems remove ice formed on the protected surfaces following a periodic cycle. One of their drawbacks of de-icing device is that ice pieces shed into the flow and may cause impact/ingestion on/in aircraft components located downstream. Aircraft manufacturers rely mainly on flight tests to evaluate the potential negative effects of ice shedding because of the lack of appropriate numerical tools. The random shape and size taken by ice shed particles together with their rotation as they move make it difficult for classical CFD tools to predict trajectories. The numerical simulation of a full unsteady viscous flow, with a set of moving bodies immersed within, shows several difficulties for grid based methods. Drawbacks income from the meshing procedure for complex geometries and the re-gridding procedure in tracing the body motion. A new approach that take into account the effect of ice accretion on flow field is used to solve the ice trajectory problem. The approach is based on mesh adaptation, penalization method and level sets.

## 4.5. ORCs cycles

ORCs are Rankine cycles that use properly chosen low-boiling molecularly heavy organic compounds to drive the turbine in place of steam. This makes them suitable for the exploitation of low grade heat sources like biomass combustion, geothermal reservoirs and heat recovery from industrial processes. ORC turbines mainly use a single (less frequently, two) stage to expand the fluid. Up till present, no experimental data are available for flows of heavy fluids in the dense gas region. Experiments are difficult because of high temperature and pressure conditions, and fluid decomposition or inflammability in presence of air. This has motivated the use of numerical simulation as a preferential tool for dense gas flow analysis, but only a limited number of papers have been devoted to the computation of dense gas flows. With no experimental validation yet available for any of these configurations, care must be taken in the analysis of the computed flow fields because of their sensitivity to the thermodynamic model and to the numerical ingredients of the discretization scheme. Since no comparison with experimental data is possible, particular attention is devoted to code validation and model assessment. We created the platform ORComp, for computing some global performance metrics, and we applied some UQ and numerical methods for taking into account the sun variability in the design of ORCs cycles, by using the platform RobUQ.

## 4.6. Atmospheric entries of spacecraft

Simulation of atmospheric entries of spacecraft is a challenging problem involving many complex physical phenomena, including rarefied gas effects, aerothermochemistry, radiation, and the response of thermal protection materials to extreme conditions. The post-flight analysis of a space mission requires accurate determination of the freestream conditions for the trajectory, that is, temperature and pressure conditions and the Mach number in front of the shock. The latter can be rebuilt from the pressure and heat flux measured on the spacecraft by means of a Flush Air Data System (FADS). This instrumentation comprises a set of sensors flush mounted in the thermal protection system to measure the static pressure (pressure taps) and heat flux (calorimeters). In this context, Computational Fluid Dynamics (CFD) supplied with UQ tools permits to take into account chemical effects and to include both measurement errors and epistemic uncertainties on the chemical model parameters in the bulk and at the wall (surface catalysis). Rebuilding the freestream conditions from the FADS data therefore amounts to solving a stochastic inverse problem. In this context, we proposed a new methodology for solving the inverse problem based on a Bayesian setting, that is, probability densities of possible values of freestream conditions are rebuilt from stagnation-point pressure and heat flux measurements. A Bayesian setting offers a rigorous foundation for inferring input parameters from noisy data and uncertain forward models, a natural mechanism for incorporating prior information, and a quantitative assessment of uncertainty on the inferred results.

## 4.7. Free surface hydrodynamics

Prediction of free surface flow hydrodynamics can be of extreme importance in many applications such as, e.g. protection of coastal environments, design of coastal structures, etc. We have developed simulation tools for the prediction of both hydrostatic and non-hydrostatic free surface flows, including also wave breaking effects. We have also started work on the improvement of the asymptotic modeling of the dispersive wave behavior which controls strongly the heights and position of the waves. These models are discretized by appropriate generalizations of the residual based techniques we propose.

In addition to the basic modeling activity, we have started to study the output dependence on the variability of input data depending on the model (such as for example, for the friction coefficient), and on environmental conditions (topography, incoming wave description etc). These quantities often involve a certain degree of uncertainty. By coupling a robust shallow-water solver based on a residual distribution scheme with some stochastic methods to show the large variability of important physical outputs (e.g. wave runup, flooded area, etc) due to input uncertainties.

## **4.8. Self healing composite materials**

In a collaboration with the UMR LCTS we are studying the influence of the in-crack physico-chemistry on the lifetimes of self healing composite materials. The self healing character of these materials is given by the presence of a reactive phase in the composite matrix which reacts with oxygen and yields a liquid oxide with a very high specific volume (compared to the reactive). The extra volume occupied by the oxide gives a protecting layer shielding the composite fibers from farther oxidation. The failure mechanism of these materials is thus strongly dependent on the evolution of this oxide.

Our objective is to develop a simplified asymptotic model of the physics and chemistry of a single crack, to be used as a numerical closure model for structural mechanics computations. This model as to provide time integrated values of oxygen concentrations at fibers, which can be used to infer fiber weakening and rupture, thus to change the crack topology. This process can be iterated until failure is obtained. Our contribution consists in developing the chemistry and flow models, related discretization, and implementation in an ad-hoc module which will be coupled with the structural solver of LCTS.

## CAGIRE Team

# 4. Application Domains

## 4.1. Effusion cooling of aeronautical combustion chambers walls

The industrial applications of our project is the cooling of the walls of the combustion chambers encountered in the helicopter engines, and more precisely, we wish to contribute to the improvement of effusion cooling.

Effusion cooling is nowadays very widespread, especially in the aeronautical context. It consists in piercing holes on the wall of the combustion chamber. These holes induce cold jets that enter inside the combustion chamber. The goal of this jet is to form a film of air that will cool the walls of the chamber, see Figure 2 .



Figure 2. Effusion cooling of aeronautical combustion chambers: close view of a typical perforated chamber wall

Effusion cooling in a combustion chamber takes at the wall where thousands of small holes allow cool air to enter inside the combustion chamber. This induces jets in crossflow in charge of cooling the walls, whatever the heat and the acoustic waves present inside the chamber. Nevertheless, this technique is not straightforward to put in practice: the size, design and position of the holes can have an important effect on the cooling efficiency. For a safe and efficient functioning of the combustion chamber, it is required that the cooling jets and the combustion effects be as much independent as possible. For example, this means that

- The jets of cool air should not mix too much with the internal flow. Otherwise it will decrease the efficiency of the combustion.
- The jets should be as much stable as possible when submitted to waves emitted in the combustion chamber, e.g. acoustic waves induced by combustion instabilities. Otherwise the jets may not cool enough the walls of the combustion chamber which can then undergoes severe damages.

The first point is what we aim at simulate in this project. As the model chosen is the fully compressible Navier Stokes system, there should not be any problem in the future for being able to simulate the effect of an acoustic forcing on the jet in crossflow.

Having a database of Direct Numerical Simulations is also fundamental for testing closure laws that are used in turbulence models encountered in RANS and LES models. With such models, it is possible for example to perform optimisation.



An important aspect that we began to address in this project is the interaction between the flow and the wall. The aim is to understand the effect of coupling between the heat propagation in the wall and the flow near the wall. A careful study of this interaction can allow to determine the exchange coefficients, and so the efficiency of the cooling by the jet. Such determination may be particularly useful to develop one or multidimensional models of wall-fluid interaction [19]. The large eddy simulation performed by Florenciano [18] clearly put into evidence the strong effect of the presence of an acoustic wave in the crossflow on the dynamics of the heat transfer coefficient at the wall.

From the application point of view, compressibility effects must be taken into account since the Mach number of the flow can reach values equal to 0.3, hence/or acoustic waves may be present inside the combustion chamber. This can raise a problem, because upwind numerical schemes are known to be less accurate in the low Mach limit.

## **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.

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

## IPSO Project-Team

### 4. Application Domains

#### 4.1. Laser physics

Laser physics considers the propagation over long space (or time) scales of high frequency waves. Typically, one has to deal with the propagation of a wave having a wavelength of the order of  $10^{-6}m$ , over distances of the order  $10^{-2}m$  to  $10^4m$ . In these situations, the propagation produces both a short-scale oscillation and exhibits a long term trend (drift, dispersion, nonlinear interaction with the medium, or so), which contains the physically important feature. For this reason, one needs to develop ways of filtering the irrelevant high-oscillations, and to build up models and/or numerical schemes that do give information on the long-term behavior. In other terms, one needs to develop high-frequency models and/or high-frequency schemes.

Generally speaking, the demand in developing such models or schemes in the context of laser physics, or laser/matter interaction, is large. It involves both modeling and numerics (description of oscillations, structure preserving algorithms to capture the long-time behaviour, etc).

In a very similar spirit, but at a different level of modelling, one would like to understand the very coupling between a laser propagating in, say, a fiber, and the atoms that build up the fiber itself.

The standard, quantum, model in this direction is called the Bloch model: it is a Schrödinger like equation that describes the evolution of the atoms, when coupled to the laser field. Here the laser field induces a potential that acts directly on the atom, and the link between this potential and the laser itself is given by the so-called dipolar matrix, a matrix made up of physical coefficients that describe the polarization of the atom under the applied field.

The scientific objective here is twofold. First, one wishes to obtain tractable asymptotic models that average out the high oscillations of the atomic system and of the laser field. A typical phenomenon here is the *resonance* between the field and the energy levels of the atomic system. Second, one wishes to obtain good numerical schemes in order to solve the Bloch equation, beyond the oscillatory phenomena entailed by this model.

#### 4.2. Molecular Dynamics

In classical molecular dynamics, the equations describe the evolution of atoms or molecules under the action of forces deriving from several interaction potentials. These potentials may be short-range or long-range and are treated differently in most molecular simulation codes. In fact, long-range potentials are computed at only a fraction of the number of steps. By doing so, one replaces the vector field by an approximate one and alternates steps with the exact field and steps with the approximate one. Although such methods have been known and used with success for years, very little is known on how the "space" approximation (of the vector field) and the time discretization should be combined in order to optimize the convergence. Also, the fraction of steps where the exact field is used for the computation is mainly determined by heuristic reasons and a more precise analysis seems necessary. Finally, let us mention that similar questions arise when dealing with constrained differential equations, which are a by-product of many simplified models in molecular dynamics (this is the case for instance if one replaces the highly-oscillatory components by constraints).

#### 4.3. Plasma physics

The development of efficient numerical methods is essential for the simulation of plasmas and beams at the kinetic level of description (Vlasov type equations). It is well known that plasmas or beams give rise to small scales (Debye length, Larmor radius, gyroperiod, mean free path...) which make numerical simulations challenging. Instead of solving the limit or averaged models by considering these small scales equal to zero, our aim is to explore a different strategy, which consists in using the original kinetic equation. Specific numerical scheme called "Asymptotic Preserving" scheme is then built to discretize the original kinetic

equation. Such a scheme allows to pass to the limit with no stability problems, and provide in the limit a consistent approximation of the limit or average model. A systematic and robust way to design such a scheme is the micro-macro decomposition in which the solution of the original model is decomposed into an averaged part and a remainder.

## MC2 Project-Team

# 4. Application Domains

## 4.1. Introduction

We now present our contribution to these above challenges concerning interface problem for complex fluids, direct simulations and analysis, flow control and optimization. From the technical point of view, many productions are common to the different parts of the project. For example, level-set methods, fast-marching procedure are used for shape optimization and for microfluidics, penalization methods are used for high Reynolds flows and for tumor growth. This leads to a strong politic of development of numerical modules.

## 4.2. Multi-fluid flows

- computation of bifluid flows : see the thesis of S. Tancogne ([78]) and P. Vigneaux ([81]). Stability of an interface, shape of droplets, formation of a jet. Study of the Plateau-Rayleigh instability. Behaviour of diphasic fluids evolving in square microchannels.
- mixing in micro-channel : see the thesis of J. Dambrine [62]. Passive mixing strategies involving boundary conditions. Enhanced oil recovery (study of mixing oil-water-polymer in a microchannel).
- emulsions and foam : see the thesis of S. Benito [47]. Applications in biology : behaviour of tissues, of tumor,....
- polymer nanotube conglomerate wire : it was the subject of a talk in the following conference "WCCM8-ECCOMAS2008" and of the talk [60].

## 4.3. Cancer modeling

- specific models : investigation of particular cancers : gliomas (brain tumors), meningioma, colorectal cancers lung and liver metastasis, breast cancer. This is one part of the PhD works of P. Berment, J. Jouganous, G. Lefebvre and post-doc of J. Joie.
- modelling of electrochemotherapy : see ARC C3MB (<http://www.math.u-bordeaux1.fr/ArcC3MB/>)
- parameter estimations with the help of low order models : see the PhD of J. Jouganous.
- patient-specific simulations
- optimal shape design : the goal is to recover the vascularization of a model tumor from the knowledge of its shape evolution.
- Theoretical biology of the metastatic process: dynamics of a population of tumors in mutual interactions, dormancy, pre-metastatic and metastatic niche, quantification of metastatic potential and differential effects of anti-angiogenic therapies on primary tumor and metastases.
- Mathematical models for preclinical cancer research: description and prediction of tumor growth and metastatic development.

## 4.4. Newtonian fluid flows simulations and their analysis

- simulation of a synthetic or pulsed jet. This is an ongoing project with Renault and PSA inside a PREDIT project.
- vortex dynamics : see [64].
- simulation of compressible flows on cartesian grids : see the thesis of Gabriele Ottino's Thesis [74], who underwent his doctoral studies in conjunction in the MC2 team and at the Politecnico di Torino, and defended in April 2009. He had a grant of the French-Italian university.



- 3D turbulent flows through DESGRIVRE contract with AIRBUS. Thesis of C. Wervaecke [83]. The goal is to use Detached-Eddy Simulation to model turbulent flows around iced bodies.
- porous media : Numerical study of coupling between Richards and transport-diffusion equations in permeable sediment affected by tidal oscillation. See the thesis of R. Chassagne [58].
- Modeling and numerical simulation of the flow around a real wind turbine. Phd thesis of Xin Jin. This includes reduced order model to design more efficient blades.

#### **4.5. Flow control and shape optimization**

- passive control : the idea is to put a porous interface between the solid body and the fluid. See the D. Depeyras thesis [63] and Yong-Liang Xiang [85] and CH Bruneau and Iraj Mortazavi) [50]. See also project [55] founded by the European Community.
- active control : see the three PhD thesis: M. Buffoni, J. Weller [82], E. Lombardi and FFAST project funded by EU and iled by the University of Bristol and AIRBUS UK.
- shape optimization for turbo-machines : See [79].
- reduced order models : it consists in designing a non-linear observer that estimates the state of the flow field from a limited number of measurements in the field. The challenge is to reduce as much as possible the information required and to take it from the boundary. See J. Weller [82] and E. Lombardi.
- passive control of flows with porous media : see [52], [49], [48], [73], [53].
- inverse problems in imagery : see [57].

## MOKAPLAN Exploratory Action

### 4. Application Domains

#### 4.1. Continuous models in Economy

- As already mentioned the CFD formulation is a limit case of simple variational Mean-Field Games (MFG) [55]. MFG is a new branch of game theory recently developed by J-M. Lasry and P-L. Lions. MFG models aim at describing the limiting behavior of stochastic differential games when the number of players tends to infinity. They are specifically designed to model economic problems where a large number of similar interacting agents try to maximize/minimize a utility/cost function which takes into account global but partial information on the game. The players in these models are individually insignificant but they collectively have a significant impact on the cost of the other players. Dynamic MFG models often lead to a system of PDEs which consists of a backward Hamilton-Jacobi Bellman equation for a value function coupled with a forward Fokker-Planck equation describing the space-time evolution of the density of agents.
- In microeconomics, the *principal-agent problem* [74] with adverse selection plays a distinguished role in the literature on asymmetric information and contract theory (with important contributions from several Nobel prizes such as Mirrlees, Myerson or Spence) and it has many important applications in optimal taxation, insurance, nonlinear pricing. The problem can be reduced to the maximization of an integral functional subject to a convexity constraint This is an unusual calculus of variations problem and the optimal price can only be computed numerically. Recently, following a reformulation of Carlier [11], convexity/well-posedness results of McCann, Figalli and Kim [42], connected to optimal transport theory, showed that there is some hope to numerically solve the problem for general utility functions.
- In [8] a class of games are considered with a continuum of players for which Cournot-Nash equilibria can be obtained by the minimisation of some cost, related to optimal transport. This cost is not convex in the usual sense in general but it turns out to have hidden strict convexity properties in many relevant cases. This enables us to obtain new uniqueness results and a characterisation of equilibria in terms of some partial differential equations, a simple numerical scheme in dimension one as well as an analysis of the inefficiency of equilibria. The mathematical problem has the structure of one step of the JKO gradient flow method.
- Many relevant markets are markets of indivisible goods characterized by a certain quality: houses, jobs, marriages... On the theoretical side, recent papers by Ekeland, McCann, Chiappori [34] showed that finding equilibria in such markets is equivalent to solving a certain optimal transport problem (where the cost function depends on the sellers and buyers preferences). On the empirical side, this allows for trying to recover information on the preferences from observed matching; this is an inverse problem as in a recent work of Galichon and Salanié [47] [48] Interestingly, these problems naturally lead to numerically challenging variants of the Monge-Kantorovich problem: the multi-marginal OT problem and the entropic approximation of the Monge-Kantorovich problem (which is actually due to Schrödinger in the early 30's).

#### 4.2. Finance

The Skorohod embedding problem (SEP) consists in finding a martingale interpolation between two probability measures. When a particular stochastic ordering between the two measures is given, Galichon et al [46] have shown that a very natural variational formulation could be given to a class of problems that includes the SEP. This formulation is related to the CFD formulation of the OT problem [2] and has applications to *model-free bounds of derivative prices in Finance*. It can also be interpreted as a multi marginal Optimal Mass Transportation with infinitely many marginals [69].

### 4.3. Congested Crowd motion

The volume preserving property appears naturally in this context where motion is constrained by the density of player.

- Optimal Mass Transportation and MFG theories can be an extremely powerful tool to attack some of these problems arising from spatial economics or to design new ones. For instance, various urban/traffic planning models have been proposed by Buttazzo, Santambrogio, Carlier, [9] [28] [20]) in recent years.
- Many models from PDEs and fluid mechanics have been used to give a description of *people or vehicles moving in a congested environment*. These models have to be classified according to the dimension (1D model are mostly used for cars on traffic networks, while 2D models are most suitable for pedestrians), to the congestion effects (“soft” congestion standing for the phenomenon where high densities slow down the movement, “hard” congestion for the sudden effects when contacts occur, or a certain threshold is attained), and to the possible rationality of the agents Maury et al [59] recently developed a theory for 2D hard congestion models without rationality, first in a discrete and then in a continuous framework. This model produces a PDE that is difficult to attack with usual PDE methods, but has been successfully studied via Optimal Mass Transportation techniques again related to the JKO gradient flow paradigm.

### 4.4. Astrophysics

In [44] and [25], the authors show that the deterministic past history of the Universe can be uniquely reconstructed from the knowledge of the present mass density field, the latter being inferred from the 3D distribution of luminous matter, assumed to be tracing the distribution of dark matter up to a known bias. Reconstruction ceases to be unique below those scales – a few Mpc – where multi-streaming becomes significant. Above 6 Mpc/h we propose and implement an effective Monge-Ampere-Kantorovich method of unique reconstruction. At such scales the Zel’dovich approximation is well satisfied and reconstruction becomes an instance of optimal mass transportation. After discretization into  $N$  point masses one obtains an assignment problem that can be handled by effective algorithms with not more than cubic time complexity in  $N$  and reasonable CPU time requirements. Testing against  $N$ -body cosmological simulations gives over 60% of exactly reconstructed points.

### 4.5. Image Processing and inverse problems

The Wasserstein distance between densities is the value function of the Optimal Mass Transportation problem. This distance may be considered to have "orthogonal" properties to the widely used least square distance. It is for instance quadratic with respect to dilations and translation. On the other hand it is not very sensitive to rigid transformations, [64] is an attempts at generalizing the CFD formulation in this context. The Wasserstein distance is an interesting tool for applications where distances between signals and in particular oscillatory signals need to be computed, this is assuming one understand how to transform the information into positive densities.

- Tannenbaum and co-authors have designed several variants of the CFD numerical method and applied it to warping, morphing and registration (using the Optimal Mass Transportation map) problems in medical imaging. [76] [17]
- Gabriel Peyre and co-authors [73] have proposed an easier to compute relaxation of the Wasserstein distance (the sliced Wasserstein distance) and applied it to two image processing problems: color transfer and texture mixing.
- Froese Engquist [40] use a Monge-Ampère Solver to compute the Wasserstein distance between synthetic 2D Seismic signals (After some transformations). Applications to waveform inversion and registration are discussed and simple numerical examples are presented.

## 4.6. Meteorology and Fluid models

In, [22] Brenier reviews in a unified framework the connection between optimal transport theory and classical convection theory for geophysical flows. Inspired by the numerical model proposed in [17], the starting point is a generalization of the Darcy-Boussinesq equations, which is a degenerate version of the Navier-Stokes-Boussinesq (NSB) equations. In a unified framework, he relates different variants of the NSB equations (in particular what he calls the generalized hydrostatic-Boussinesq equations) to various models involving optimal transport and the related Monge-Ampère equation. This includes the 2D semi-geostrophic equations [51] [38] [37] [4] [57] and some fully nonlinear versions of the so-called high-field limit of the Vlasov-Poisson system [65] and of the Keller-Segel system for chemotaxis [53] [33] .

## 4.7. Mesh motion/Lagrangian methods

The necessity to preserve areas/volumes is an intrinsic feature of mesh deformations more generally Lagrangian numerical methods. Numerical method of Optimal Mass Transportation which preserve some notions of convexity and as a consequence the monotonicity of the computed transport maps can play a role in this context, see for instance [32] [35] [56].

## 4.8. Density Functionnal Theory (DFT)

The precise modeling of electron correlations continues to constitute the major obstacle in developing high-accuracy, low-cost methods for electronic structure computations in molecules and solids. The article [36] sheds a new light on the longstanding problem of how to accurately incorporate electron correlation into DFT, by deriving and analyzing the semiclassical limit of the exact Hohenberg-Kohn functional with the single-particle density  $\rho$  held fixed. In this limit, in the case of two electrons, the exact functional reduces to a very interesting functional that depends on an optimal transport map  $M$  associated with a given density  $\rho$ . The limit problem is known in the DFT literature with the optimal transport map being called a correlation function or a co-motion function , but it has not been rigorously derived, and it appears that it has not previously been interpreted as an optimal transport problem. The article [36] thereby links for the first time DFT, which is a large and very active research area in physics and chemistry, to optimal transportation theory, which has recently become a very active area in mathematics. Numerics are still widely open [26].

## **NACHOS Project-Team**

# **4. Application Domains**

## **4.1. Computational electromagnetics**

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.).

Part of the activities of the NACHOS project-team aim at the development of high performance, high order, unstructured mesh based solvers for the full system of Maxwell equations, in the time domain and frequency domain regimes. Although many of the above-mentioned electromagnetic wave propagation problems can potentially benefit from the proposed numerical methodologies, the team concentrates its efforts on the following two situations.

### ***4.1.1. Interaction of electromagnetic waves with biological tissues at microwave frequencies.***

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 [63]. 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 [15].



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. Interaction of electromagnetic waves with nanoparticles at optical frequencies (nanophotonics).

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. Nanostructures whose optical scattering is dominated by the response of the conduction electrons are considered as plasmomic media. If the structure presents an interface with e.g. a dielectric with a positive permittivity, collective oscillations of surface electrons create surface-plasmons-polaritons (SPPs) that propagate along the interface. SPPs are guided along metal-dielectric interfaces much in the same way light can be guided by an optical fiber, with the unique characteristic of subwavelength-scale confinement perpendicular to the interface. Nanofabricated systems that exploit SPPs offer fascinating opportunities for crafting and controlling the propagation of light in matter. In particular, SPPs can be used to channel light efficiently into nanometer-scale volumes, leading to direct modification of mode dispersion properties (substantially shrinking the wavelength of light and the speed of light pulses for example), as well as huge field enhancements suitable for enabling strong interactions with nonlinear 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 [49]- [64].

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 the Drude and Drude-Lorentz models. Her 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 [54]- [56]- [47]. The activities of the NACHOS project-team towards the development of accurate and efficient unstructured mesh based methods for nanophotonic applications have started in 2012 and are conducted in collaboration with Dr. Maciej Klemm at University of Bristol who is designing nanoantennas for medical applications [55].

## **4.2. Computational geoseismics**

Computational challenges in geoseismics span a wide range of disciplines and have significant scientific and societal implications. Two important topics are mitigation of seismic hazards and discovery of economically recoverable petroleum resources. The research activities of the NACHOS project-team in this domain before all focus on the development of numerical methodologies and simulation tools for seismic hazard assessment, while the involvement on the second topic has been initiated recently.



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 (PhD thesis of Jonathan Viquerat).



#### 4.2.1. Seismic hazard assessment.

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 building codes 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 multi-scale 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. Modeling and forecasting earthquake ground motion in large basins is a challenging and complex task. The complexity arises from several sources. First, multiple scales characterize the earthquake source and basin response: the shortest wavelengths are measured in tens of meters, whereas the longest measure in kilometers; basin dimensions are on the order of tens of kilometers, and earthquake sources up to hundreds of kilometers. Second, temporal scales vary from the hundredths of a second necessary to resolve the highest frequencies of the earthquake source up to as much as several minutes of shaking within the basin. Third, many basins have a highly irregular geometry. Fourth, the soil's material properties are highly heterogeneous. And fifth, geology and source parameters are observable only indirectly and thus introduce uncertainty in the modeling process. Because of its modeling and computational complexity, earthquake simulation is currently recognized as a grand challenge problem.

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 [62] and based on the first order velocity-stress hyperbolic system of elastic waves equations, which is an extension of the scheme derived by Yee [63] 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 [2]-[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.

#### 4.2.2. Imperfect interfaces.

A long term scientific collaboration (at least 5 years long) has been recently set up between the NACHOS project-team and LMA (Laboratoire de Mécanique et Acoustique) <http://www.lma.cnrs-mrs.fr> with the arrival of Marie-Hélène Lallemand who joined NACHOS in October 2012. That collaboration has been motivated by common scientific interests concerning both geodynamics (seismic wave propagation) and seismology (Non Destructive Control by wave propagation). The goal is to contribute in the area of both fracture dynamics modelings and the setting of adequate constitutive laws for interfaces separating two continuous media. Since the whole medium under study is heterogeneous in term of both materials and geometries, the study of



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

equivalent homogeneous representation/modellings is crucial to get a suitable reduced model which can be used for numerical simulations. In the particular example of rock-type soils near mountain areas, the medium may be viewed from the geologist, at the macro-scale, for example, as large layers of continuous materials separated by interfacial areas through which discontinuities (of displacements, velocities, stress components ...) may occur. Even if the so-called interfaces may have a depth which may attain many times ten meters and a length of many times hundred meters, they are assimilated as interfaces, from the geologist point of view. Inside those *thin* layers, there are usually some mixture of multiphase materials (water, sand, gas, etc.), and the exact composition is not known in advance. While perfect interfaces are usually assumed in inverse problems in sismology, the question is to qualify and to quantify the errors if we do not take those assumptions for granted. When soil rheology is requested, assuming perfect interfaces or imperfect interfaces greatly influence the physical parameters obtained in reversing the data collected in the captors. Interface modelling is one of the expertise area of LMA, and the project-team is interested in taking that opportunity to improve its knowledge in multi-scale modelling while ready to help answering the numerical implementation of such resulting models. That collaboration is not restricted to that aspect though. Well-posedness of the resulting models, numerical solvers are also domains which are also addressed.

### 4.2.3. 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 Team

### 3. Application Domains

#### 3.1. 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.

#### 3.2. 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.

#### 3.3. 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.

### 3.4. 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.*

The magazine Science has recently featured a paper demonstrating an example of DNA nanotechnology, where DNA strands are stacked together through programmable self-assembly. In February 2007, the cover of Nature Nanotechnology showed a “nano-wheel” composed of a few atoms only. Several nanosystems have already been demonstrated, including a wheelbarrow molecule, a nano-car and a Morse molecule, etc. Typically, these nanosystems are designed in part *via* quantum mechanics calculations, such as the semi-empirical ASED+ calculation technique.

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



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

We have recently shown 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).

## OPALE Project-Team

### 4. Application Domains

#### 4.1. Aeronautics and space

The demand of the aeronautical industry remains very strong in aerodynamics, as much for conventional aircraft, whose performance must be enhanced to meet new societal requirements in terms of economy, noise (particularly during landing), vortex production near runways, etc., as for high-capacity or supersonic aircraft of the future. Our implication concerns shape optimization of wings or simplified configurations.

Our current involvement with Space applications relates to software platforms for code coupling.

#### 4.2. Mechanical industry

A new application domain related to the parameter and shape optimization of mechanical structures is under active development. The mechanical models range from linear elasticity of 2D or 3D structures, or thin shells, to nonlinear elastoplasticity and structural dynamics. The criteria under consideration are multiple: formability, stiffness, rupture, fatigue, crash, and so on. The design variables are the thickness and shape, and possibly the topology, of the structures. The applications are performed in collaboration with world-leading industrials, and involve the optimization of the stamping process (Blank Force, Die and Tools shapes) of High Performance steel structures as well as the optimal design of structures used for packaging purposes (cans and sprays under high pressure). Our main contribution relies on providing original and efficient algorithms to capture Pareto fronts, using smart meta-modelling, and to apply game theory approaches and algorithms to propose stable compromise solutions (e.g. Nash equilibria).

#### 4.3. Electromagnetics

In the context of shape optimization of antennas, we can split the existing results in two parts: the two-dimensional modeling concerning only the specific transverse mode TE or TM, and treatments of the real physical 3-D propagation accounting for no particular symmetry, whose objective is to optimize and identify real objects such as antennas.

Most of the numerical literature in shape optimization in electromagnetics belongs to the first part and makes intensive use of the 2-D solvers based on the specific 2-D Green kernels. The 2-D approach for the optimization of *directivity* led recently to serious errors due to the modeling defect. There is definitely little hope for extending the 2-D algorithms to real situations. Our approach relies on a full analysis in unbounded domains of shape sensitivity analysis for the Maxwell equations (in the time-dependent or harmonic formulation), in particular, by using the integral formulation and the variations of the Colton and Kreiss isomorphism. The use of the France Telecom software SR3D enables us to directly implement our shape sensitivity analysis in the harmonic approach. This technique makes it possible, with an adequate interpolation, to retrieve the shape derivatives from the physical vector fields in the time evolution processes involving initial impulses, such as radar or tomography devices, etc. Our approach is complementary to the “automatic differentiation codes” which are also very powerful in many areas of computational sciences. In Electromagnetics, the analysis of hyperbolic equations requires a sound treatment and a clear understanding of the influence of space approximation.

#### 4.4. Biology and medicine

A particular effort is made to apply our expertise in solid and fluid mechanics, shape and topology design, multidisciplinary optimization by game strategies to biology and medicine. We focus more precisely on developing and validating cell dynamics models. Two selected applications are privileged: solid tumors and wound healing.

Opale's objective is to push further the investigation of these applications, from a mathematical-theoretical viewpoint and from a computational and software development viewpoint as well. These studies are led in collaboration with biologists, as well as image processing specialists.

#### **4.5. Traffic flow**

The modeling and analysis of traffic phenomena can be performed at a macroscopic scale by using partial differential equations derived from fluid dynamics. Such models give a description of collective dynamics in terms of the spatial density  $\rho(t, x)$  and average velocity  $v(t, x)$ . Continuum models have shown to be in good agreement with empirical data. Moreover, they are suitable for analytical investigations and very efficient from the numerical point of view. Finally, they contain only few variables and parameters and they can be very versatile in order to describe different situations encountered in practice.

Opale's research focuses on the study of macroscopic models of vehicular and pedestrian traffic, and how optimal control approaches can be used in traffic management. The project opens new perspectives of interdisciplinary collaborations on urban planning and crowd dynamics analysis.

#### **4.6. Multidisciplinary couplings**

Our expertise in theoretical and numerical modeling, in particular in relation to approximation schemes, and multilevel, multi-scale computational algorithms, allows us to envisage to contribute to integrated projects focused on disciplines other than, or coupled with fluid dynamics, such as structural mechanics, electromagnetics, biology and virtual reality, image processing, etc in collaboration with specialists of these fields. Part of this research is conducted in collaboration with ONERA.

## POEMS Project-Team

# 4. Application Domains

## 4.1. Introduction

We are concerned with all application domains where linear wave problems arise: acoustics and elastodynamics (including fluid-structure interactions), electromagnetism and optics, and gravity water waves. We give in the sequel some details on each domain, pointing out our main motivations and collaborations.

## 4.2. Acoustics

As the acoustic propagation in a fluid at rest can be described by a scalar equation, it is generally considered by applied mathematicians as a simple preliminary step for more complicated (vectorial) models. However, several difficult questions concerning coupling problems have occupied our attention recently. Aeroacoustics, or more precisely, acoustic propagation in a moving compressible fluid, is for our team a new and very challenging topic, which gives rise to a lot of open questions, from the modelling (Euler equations, Galbrun equations, Goldstein equation) to the numerical approximation of such models (which poses new difficulties). Our works in this area are partially supported by EADS and Airbus. The typical objective is to reduce the noise radiated by Airbus planes. Vibroacoustics, which concerns the interaction between sound propagation and vibrations of thin structures, also raises up a lot of relevant research subjects.

Both applications (aeroacoustics and vibroacoustics) led us in particular to develop an academic research between volumic methods and integral equations in time domain.

Finally, a particularly attractive application concerns the simulation of musical instruments, whose objectives are both a better understanding of the behavior of existing instruments and an aid for the manufacturing of new instruments. The modelling and simulation of the timpani, the guitar and the piano have been carried out in collaboration with A. Chaigne of ENSTA. This work will continue in the framework of the European Project BATWOMAN.

## 4.3. Electromagnetism

This is a particularly important domain, first because of the very important technological applications but also because the treatment of Maxwell's equations is much more technically involved from the mathematical point of view than the scalar wave equation. Applied mathematics for electromagnetism during the last ten years have mainly concerned stealth technology, electromagnetic compatibility, design of optoelectronic micro-components or smart materials. Stealth technology relies in particular on the conception and simulation of new absorbing materials (anisotropic, chiral, non-linear...). The simulation of antennas raises delicate questions related to the complexity of the geometry (in particular the presence of edges and corners). In optics, the development of the micro and nano optics has made recently fantastic progress and the thematic of metamaterials (with negative index of refraction) opens new amazing applications. For all these reasons, we are developing an intense research in the following areas

- Highly accurate and hybrid numerical methods in collaboration with CEA (Gramat) and ONERA (Toulouse).
- Electromagnetic wave propagation in periodic media.
- Development of simplified approximate models by asymptotic analysis for various applications : boundary layers, thin coatings, thin domains, thin wires and cables, ...
- Mathematical and numerical questions linked to the modeling of metamaterials.



## **4.4. 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.

Our activity on this topic began with applications in geophysics, which unfortunately has been forced to slow down in the middle of the 90's due to the disengagement of French oil companies in matter of research. However it has seen a most welcomed rebound through new academic problems (in particular surface waves, perfectly matched layers techniques, inverse problems in wave guides) and industrial contacts, more precisely with CEA-LIST with which we have developed a long term collaboration in the domain of non destructive testing by ultrasounds. The most recent problems we have been dealing with in this domain concern elastic wave propagation in plates, the modeling of piezoelectric devices or elastic wave propagation in highly heterogeneous media.

## APICS Project-Team

# 4. Application Domains

## 4.1. Introduction

These 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 described in Section 3.3 .

## 4.2. Inverse source problems in EEG

**Participants:** Laurent Baratchart, Kateryna Bashtova, Juliette Leblond.

This work is done in collaboration with Maureen Clerc and Théo Papadopoulo from the Athena Project-Team, and Jean-Paul Marmorat (Centre de mathématiques appliquées - CMA, École des Mines de Paris).

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 since the latter involves propagating the initial conditions through several layers of different conductivities, from the boundary down to the center of the domain where the singularities (*i.e.* the sources) lie. Then, once propagated to the innermost sphere, it turns out that that traces of the boundary data on 2-D cross sections (disks) coincide with analytic functions in the slicing plane, that has branched singularities inside the disk [3]. These singularities are related to the actual location of the sources (namely, they reach in turn a maximum in modulus when the plane contains one of the sources). Hence, we are back to the 2-D framework of Section 3.3.3 where approximately recovering these singularities can be performed using best rational approximation. The goal is to produce a fast but already good enough 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 give very good results on simulated data and we are now engaged in the process of handling real experimental magneto-encephalographic data, see also Sections 5.6 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, Dmitry Ponomarev.

Generally speaking, inverse potential problems similar to the one in Section 4.2 appear 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, whose study led us to form an Inria Associate Team ("IMPINGE" for Inverse Magnetization Problems IN GEosciences) together with MIT and Vanderbilt University.

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 submillimeter 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, from Maxwell's equations. The big 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 [14] and Section 6.1.2 .

#### 4.4. Free boundary problems

**Participants:** Laurent Baratchart, Juliette Leblond, Slah Chaabi.

The team has engaged in the study of problems with variable conductivity  $\sigma$ , governed by a 2-D equation of the form  $\operatorname{div}(\sigma \nabla u) = 0$ . Such equations are in one-to-one correspondence with real parts of solutions to conjugate-Beltrami equations  $\bar{\partial} f = \nu \partial \bar{f}$ , so that complex analysis is a tool to study them, see [4], [13], [28]. This research was prompted by issues in plasma confinement for thermonuclear fusion in a tokamak, more precisely with the extrapolation of magnetic data on the boundary of the chamber from the outer boundary of the plasma, which is a level curve for the poloidal flux solving the original div-grad equation. Solving this inverse problem of Bernoulli type is of importance to determine the appropriate boundary conditions to be applied to the chamber in order to shape the plasma [58]. This research was started in collaboration with CEA-IRFM (Cadarache) and the Laboratoire J.-A. Dieudonné at the Univ. of Nice-SA. Within the team, it is now expanding to cover Dirichlet-Neumann problems for larger classes of conductivities, *cf.* in particular, the PhD thesis of S. Chaabi [12], [28], jointly supervised with the CMI-LATP at the Aix-Marseille University. (see Section 6.2 ).

#### 4.5. Identification and design of microwave devices

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

This work is done in collaboration with Stéphane Bila (XLIM, Limoges) and Jean-Paul Marmorat (Centre de mathématiques appliquées (CMA), École des Mines de Paris).

One of the best training grounds for the research of the team in function theory is the identification and design of physical systems for which the linearity assumption works well in the considered range of frequency, and whose specifications are made in the frequency domain. 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 essentially only a discrete set of wave vectors is selected. In the considered range of frequency, the electrical field in each cavity can be seen as being 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).



*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.*

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 the screws are conductors, they act more or less 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 the iris is to the contrary of a screw: no condition is imposed where there is 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. 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 of the Maxwell equations is given by the solution of a second order differential equation. One obtains thus an electrical model for our filter as a sequence of electrically-coupled resonant circuits, and each circuit will be modeled by two resonators, one per mode, whose resonance frequency represents the frequency of a mode, and whose resistance represent the electric losses (current on the surface).

In this way, the filter can be seen as a quadripole, with two ports, when plugged on a resistor at one end and fed with some potential at the other end. We are then interested in the power which is transmitted and reflected. This leads to defining a scattering matrix  $S$ , that can 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), and the key step consists in expressing the components of the equivalent electrical circuit as a function of the  $S_{i,j}$  (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 design, particularly 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 not have real coefficients) but whose degree is divided by 2 (8 in the example).

In short, the identification strategy 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).

The final approximation is of high quality. This can be interpreted as a validation of the linearity hypothesis for 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, useful for the synthesis of repeating devices.



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

The team also investigates problems relative to the design of optimal responses for microwave devices. The resolution of a quasi-convex Zolotarev problems was for example proposed, in order to derive guaranteed optimal multi-band filter's responses subject to modulus constraints [10]. This generalizes the classical single band design techniques based on Chebyshev polynomials and elliptic functions. These techniques rely on the fact that the modulus of the scattering parameters of a filters, say  $|S_{1,2}|$ , 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 and 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 is due to the possibility of "forgetting" about Feldtkeller's equation, and express all design constraints in terms of the filtering function  $D$ . 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 one of the team's active recent research area, where techniques based on constrained Nevanlinna-Pick interpolation problems are being considered (see Section 6.3.1 ).

## 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.

## 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.

## 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. Optimization

Optimization exists in virtually all economic sectors. Simulation tools can be used to optimize the simulated system. Another domain is parameter *identification* (Idopt or Estime teams), where the deviation between measurements and theoretical predictions must be minimized. Accordingly, giving an exhaustive list of applications is impossible. Some domains where Inria has been involved in the past, possibly through the former Promath and Numopt teams are: production management, geophysics, finance, molecular modeling, robotics, networks, astrophysics, crystallography, ...Our current applicative activity includes: the management of electrical production (deterministic or stochastic), the design and operation of telecommunication networks.

## **4.5. 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 have just started to study certain discrepancies (inexistence of solution) due to the combination of incompatible models such as contacting rigid bodies subject to Coulomb friction.



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

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

## **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 [49]). 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 [31],
- bounds on the controllability time [27],
- STIRAP processes [99],
- simultaneous control [72],
- optimal control ([68], [40], [51]),
- 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, [32], [69], [90], [46]).

In the case where the state space is infinite dimensional, some optimal control results are known (see, for instance, [36], [47], [65], [37]). 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 [38], [39] 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], [43].

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 [35], [48]. 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 [34]), 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 [41], [42], [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], [28].

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 [44].

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 (section vide)**



## Maxplus Project-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 [126], pour des réseaux ferroviaires [76] ou routiers, et l'évaluation de performance des réseaux de communication [66]. 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" [70], [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 [143], [140], [102].

##### *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 [126] 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 [66]. 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 [70], [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 [143], [140], [102].

#### 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 [176]. 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 [112] pour le cas du “jobshop”, une représentation plus simple a été obtenue dans [137] 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 [137]. 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 [176]. 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 [112] for the jobshop case, a simpler representation was given in [137] 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 [137]. 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
}

```

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

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], [109], 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 [166]). 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 [110], [83], [84],[7]. Une version assez générale de cet algorithme, adaptée au domaine des templates, est décrite dans [109] 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], [109], 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 [166]). 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 [110], [83], [84],[7]. A rather general version of this policy iteration algorithm, adapted to the domain of templates, is described in [109], 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>2</sup>.

#### 4.1.4. Context for these applications

The geographic proximity of Thales Alenia Space, in conjunction with the “Pole de compétitivité” PEGASE in PACA region is an asset for a long term collaboration between Inria - Sophia Antipolis and Thales Alenia Space (Thales Alenia Space site located in Cannes hosts one of the very few European facilities for assembly, integration and tests of satellites).

B. Bonnard and J.-B. Caillau in Dijon have had a strong activity in optimal control for space, in collaboration with the APO Team from IRIT at ENSEEIHT (Toulouse), and sometimes with EADS, for development of geometric methods in numerical algorithms.

## 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

<sup>2</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.

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) [31], [30].

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 [29]; 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.

Note that a reference book by B. Bonnard and D. Sugny has been published on the topic [32].

### 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. Two more specific fields:

- 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 [57].
- 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 [59] in the GEOMETRICA project-team. The relevant distance between measures is again the one coming from optimal transportation.
- A collaboration between Ludovic Rifford and Robert McCann from the University of Toronto aims at applications of optimal transportation to the modeling of markets in economy; it was to subject of Alice Erlinger’s PhD, unfortunately interrupted.

Applications *specific to the type of costs that we consider*, 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 [47]; also, closed geodesics for perturbed Riemannian metrics were constructed in [50], [51] using control techniques.

The work in progress [39] 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. Also, in [65], L. Rifford and R. Ruggiero applied successfully geometric control techniques to obtain genericity properties for Hamiltonian 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.
- Pedestrian navigation, providing guidance e.g. to first responders after a disaster, or to blind people walking in unfamiliar environments. This task is particularly challenging in-door, where no GPS is available.
- 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 Sect. 5.1 and <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 [44], 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. 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. On-going research in the team concerns source localization, with a fleet of mobile robots, including wheeled land vehicles.

## NON-A Project-Team

### 4. Application Domains

#### 4.1. Networked robots

Both economically and scientifically, cooperation in robot swarms represents an important issue since it concerns many service applications (health, handicap, urban transports...) and can increase the potential of sensor networks <sup>4</sup>. It involves several challenges such as:

- Because autonomy is a key for being able to increase the network size, maximize the autonomy of the robots in their different tasks of localization, motion, communication;
- Aiming at making 1+1 be more than 2, extend the global potential of the swarm by introducing collaboration (exchanging information with other robots) and cooperation (acting with other robots);
- Include time and energy saving considerations at the design stage.

The self deployment of autonomous groups of mobile robots in an unknown environment (including different kinds of static or moving obstacles) involves localization, path planning and robust control problems. Both the control and signal aspects of our researches are oriented to solve some problems coming from – or taking advantage of – such collaboration frameworks. To mention a few:

- Localization using as few as possible landmarks and exteroceptive information by means of derivative estimates;
- Image-based sensing algorithms inspired by our multidimensional estimation techniques;
- Detection and adaptation to sudden loss of communication, time-varying topology, or communication delays;
- Robust, autonomous, energy-aware controllers based on either model-free or model-based techniques.

Several algorithms have already been applied to the control of formations of mobile robots: an illustrative platform is currently developed at EuraTechnologie center within the framework of *Non-A*<sup>5</sup>. They are now being extended to medical devices (such as wheelchairs) within the European project *SYSIASS* (see <http://www.sysiass.eu>), in collaboration with partners from hospital settings.

Another future application concerns Wireless Sensor and Robot Networks (WSRN, Fig. 2 ), dedicated to the surveillance of zones, to the exploration of hostile areas, or to the supervision of large scale sensor networks. The main idea here is to integrate mobile nodes (the mobile robots) within the sensor network, allowing to overcome a sensor defection, to maintain the connectivity of the network, or to extend the coverage area during a random deployment. This involves consideration about mobile actuators within a mobile network of sensors and control networks (wireless) with strong constraints on the possibilities of communication in a noisy and non-homogeneous environment. This work is made in close collaboration with the Inria project-team *POPS* (Lille), which brings its expertise in terms of sensor networks. It takes place in the framework of the Inria ADT *SENSAS* and represents our contribution to the LABEX proposal *ICON*.

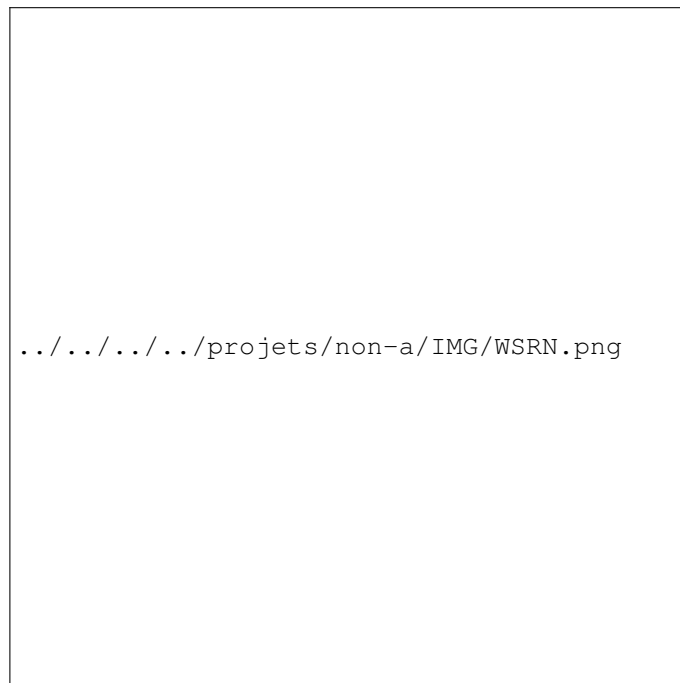
#### 4.2. Nano/macro machining

*Nano machining:*

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<sup>4</sup>Integrating wireless sensor networks and multi-robot systems increases the potential of the sensors: robots, in comparison, are resource-rich and can be involved in taking decisions and performing appropriate actions on themselves on sensors and/or the environment.

<sup>5</sup>“RobotCity” was exhibited for the first time during the opening ceremony held on April 6th, 2011



*Figure 2. An illustration of collaboration in a Wireless Sensor and Robot Network.*

Recent research investigations have reported the development of a number of process chains that are complementary to those used for batch manufacturing of Micro Electro Mechanical Systems (MEMS) and, at the same time, broaden the application domain of products incorporating micro and nano scale features. Such alternative process chains combine micro and nano structuring technologies for master making with replication techniques for high volume production such as injection moulding and roll-to-roll imprinting. In association with the Manufacturing Engineering Center of Cardiff, Arts et Metiers ParisTech center of Lille develops a new process chain for the fabrication of components with nano scale features. In particular, AFM probe-based nano mechanical machining is employed as an alternative master making technology to commonly used lithography-based processes (Fig. 3 ). Previous experimental studies demonstrated the potential of this approach for thermoplastic materials. Such a manufacturing route also represents an attractive prototyping solution to test the functionalities of components with nano scale features prior to their mass fabrication and, thus, to reduce the development time and cost of nano technology-enabled products. Application of our control and estimation techniques improves the trajectory tracking accuracy and the speed of the machining tools.



Figure 3. Left: A machined nano structure:  $16\mu\text{m} \times 8\mu\text{m} \times \text{some nm}$ . Right: Nano-positioning system available at Arts et Métiers ParisTech Lille ( $75\mu\text{m}$  range of motion).

#### *Machining with industrial robots:*

Industrials are enthusiastic to replace machine-tools with industrial robots: compared to machine-tools, industrial articulated robots are very cheaper, more flexible, and exhibit more important workspaces. They can carry out machining applications like prototyping, cleaning and pre-machining of cast parts, as well as end-machining of middle tolerance parts. Such applications require high accuracy in the positioning and path tracking. Unfortunately, industrial robots have a low stiffness and are not that accurate<sup>6</sup> and they deserve an increased quality of control.

We deal with the modelling and the on-line identification of flexible-joint robot models. This can be used both for dynamic simulation and model-based control of industrial robots. We address the problem of real-time identification of the parameters involved in the dynamic linear model of an industrial robot axis. This

<sup>6</sup>Industrial robots were designed to realize repeatable tasks. The robot repeatability ranges typically from 0.03 to 0.1mm, but the accuracy is often measured to be within several millimetres. Due to their serial structure, articulated robot has lower stiffness (less than  $1\text{ N/mm}$ ) than classical machine-tools (greater than  $50\text{ N/mm}$ ). These poor accuracy and stiffness are caused by many factors, such as geometric parameter errors (manufacturing tolerances), wear of parts and components replacement, as well as flexibility of links and gear trains, gear backlashes, encoder resolution errors and thermal effects.

is possible thanks to a special sensor developed by Arts et Métiers, subject to an EADS project within the FUI (Fonds Unique Interministériel). Control algorithms for other machining actuators such as active magnet bearings are also under study. Within the framework of LAGIS, we also consider the remote control of industrial robots (via internet or Wi-Fi links, for instance), which sets numerous problems in relation with the communication delays.

### **4.3. Multicell chopper**

On the basis of benchmarks developed at ECS-lab (ENSEA Cergy), we intend to work on the control and observation of serial and parallel multicell choppers, as well as more usual power converters. These power electronic systems associated with their respective loads are typical hybrid dynamical systems and many industrial and/or theoretical challenging problems occur. For example, in the industrial problem of power supply for a supercomputer, the parallel multicell chopper appears as a new solution particularly with respect to the power efficiency. Nevertheless, the observation and control of such hybrid dynamical systems is a difficult task, where non asymptotic estimation and control can be useful.

## CLASSIC Project-Team

### 4. Application Domains

#### 4.1. Forecasting of the electricity consumption

Our partner is EDF R&D. The goal is to aggregate in a sequential fashion the forecasts made by some (about 20) base experts in order to predict the electricity consumption at a global level (the one of all French customers) at a half-hourly step. We need to abide by some operational constraints: the predictions need to be made at noon for the next 24 hours (i.e., for the next 48 time rounds).

#### 4.2. Forecasting of the air quality

Our partner is the Inria project-team CLIME (Paris-Rocquencourt). The goal is to aggregate in a sequential fashion the forecasts made by some (about 100) base experts in order to output field prediction of the concentration of some pollutants (typically, the ozone) over Europe. The results were and will be transferred to the public operator INERIS, which uses and will use them in an operational way.

#### 4.3. Forecasting of the production data of oil reservoirs

Our partner is IFP Energies nouvelles. The goal is to aggregate in a sequential fashion the forecasts made by some (about 100) base experts in order to predict some behaviors (gas/oil ratio, cumulative oil extracted, water cut) of the exploitation of some oil wells.

#### 4.4. Forecasting of exchange rates

Our partner is HEC Paris. The goal is to aggregate in a sequential fashion the forecasts made by some (about 5) base macro-economic variables to predict monthly-averaged exchange rates.

#### 4.5. Data mining, massive data sets

Our partner is the start-up Safety Line. The purpose of this application is to investigate statistical learning strategies for mining massive data sets originated from aircraft high-frequency recordings and improve security.

#### 4.6. Computational linguistics

We propose and study new language models that bridge the gap between models oriented towards the statistical analysis of large corpora and grammars oriented towards the description of syntactic features as understood by academic experts. We have conceived a new kind of grammar, based on some cut and paste mechanism and some label aggregation principle, that can be fully learnt from a corpus. We are currently testing this model and studying its mathematical properties and relations with some other new statistical models based on conditional independence assumptions.

#### 4.7. Statistical inference on biological data

The question is about understanding how interactions between neurons can be detected. A mathematical modeling is given by multivariate Hawkes processes. Lasso-type methods can then be used to estimate interaction functions in the nonparametric setting by using fast algorithms, providing inference of the unitary event activity of individual neurons.

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## DOLPHIN Project-Team

## 4. Application Domains

### 4.1. Academic Benchmark Problems

- $\rho MNK$ -landscapes [34] constitute a problem-independent model used for constructing multiobjective multimodal landscapes with objective correlation. They extend single-objective NK-landscapes [90] and multiobjective NK-landscapes with independent objective functions [85]. The four parameters defining a  $\rho MNK$ -landscape are: (i) the size of (binary string) solutions  $N$ , (ii) the variable correlation  $K < N$ , (iii) the number of objective functions  $M$ , and (iv) the correlation coefficient  $\rho$ . A number of problem instances and an instance generator are available at the following URL: <http://mocobench.sf.net/>.
- The Unconstrained Binary Quadratic Programming (UBQP) problem is known to be a unified modeling and solution framework for many combinatorial optimization problems [91]. Given a collection of  $n$  items such that each pair of items is associated with a profit value that can be positive, negative or zero, UBQP seeks a subset of items that maximizes the sum of their paired values. In [29], we proposed an extension of the single-objective UBQP to the multiobjective case (mUBQP), where multiple objectives are to be optimized simultaneously. We showed that the mUBQP problem is both NP-hard and intractable. Some problem instances with different characteristics and an instance generator are also available at the following URL: <http://mocobench.sf.net/>.

### 4.2. Transportation and logistics

- **Scheduling problems:** 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 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. Multiple combinations of two objective functions have also been investigated. At last, a three-objective flow-shop problem, minimizing in addition the maximum tardiness, is also studied. It allows us to develop and test multi-objective (and not only bi-objective) exact methods.
- **Routing problems:** 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. As far as we know, this model is one of the pioneer works in the literature. One of our current goals, related to an Inria ADT project, is to propose a VRP library called VRP-solve that is able to cope with a multiple objective and a large number of constraints. This code will be used in future industrial collaborations, and already includes algorithms to use GIS.
- **Packing problems:** In logistic and transportation fields, packing problems may be a major issue in the delivery process. They arise when one wants to minimize the size of a warehouse or a cargo, the number of boxes, or the number of vehicles used to deliver a batch of items. These problems have been the subjects of many papers, but only few of them study multi-objective cases, and to our knowledge, never from an exact point of view. Such a case occurs for example when some pairs of items cannot be packed in the same bin. The DOLPHIN project is currently studying the problem in its one-dimensional version. We plan to generalize our approach to two and three dimensional problems, and to more other conflict constraints, with the notion of *distance* between items.

### 4.3. 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.

#### 4.3.1. 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, started in 2010, 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.

#### 4.3.2. Optimization for health care

The collaboration (PhD thesis 2010-2013) 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.



## **GEOSTAT Project-Team**

# **4. Application Domains**

## **4.1. Application Domains**

In GEOSTAT, the development of nonlinear methods for the study of complex systems and signals is conducted on four broad types of complex signals:

- Ocean dynamics and ocean/atmosphere interactions: generation of high-resolution maps from cascading properties and the determination of optimal wavelets [12], geostrophic or non-geostrophic complex oceanic dynamics, mixing phenomena.
- Speech signal (analysis, recognition, classification) [15], [17].
- Optimal wavelets for phase reconstruction in adaptive optics [20], [28], [14].
- Heartbeat signals, in cooperation with IHU LIRYC and Professor M. Haissaguerre (INSERM EA 2668 Electrophysiology and Cardiac Stimulation) [34], [21].

## **MISTIS Project-Team**

### **4. Application Domains**

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

**Participants:** Christine Bakhous, Senan James Doyle, Aina Frau Pascual, Thomas Vincent, Florence Forbes, Stéphane Girard, Darren Wraith, Flor Vasseur, Alessandro Chiancone, Farida Enikeeva.

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. In the context of the ANR MDCO project Vahine, we worked on hyperspectral multi-angle 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:** Thomas Vincent, Christine Bakhous, Aina Frau-Pascual, Senan James Doyle, Florence Forbes, Stéphane Girard, Jonathan El-Methni, Gildas Mazo, Angelika Studeny, Seydou-Nourou Sylla, Marie-José Martinez, Jean-Baptise 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 population genetics and 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. Domain**

Potential application areas of statistical modeling for heterogeneous data are extensive but some particular areas are identified. For historical reasons and considering the background of the team members, MODAL is mainly focused on biological applications where new challenges in high throughput technologies are opened. In addition, other secondary applications areas are considered in industry, retail, credit scoring and astronomy. Several contacts and collaborations are already established with some partners in these application areas and are described in Sections 7 and 8.

## REALOPT Project-Team

# 4. Application Domains

## 4.1. Introduction

Our group has tackled applications in logistics, transportation and routing [75], [74], [70], [72], in production planning [94] and inventory control [70], [72], in network design and traffic routing [51], [61], [68], [97], [49], [62], [81], [87], in cutting and placement problems [77], [78], [91], [92], [93], [95], and in scheduling [5], [82], [47].

## 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 [61]. 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 [99], [98], [97] 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 [96]. 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 [68], [69].

We studied several time dependent formulations for the unit demand vehicle routing problem [53], [52]. 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 [86] 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 [21]. 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 [10] 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 [72]: we faced a multiple-class integer knapsack problem with setups [71] (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 [65], [63], [67], [66]. 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 now organizing a european challenge on packing with society Renault. This challenge will be held in 2014 and will be about loading trucks under practical constraints.

#### 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 truncated branch-and-price algorithm: periodic plans are generated for vehicles by solving a multiple choice knapsack subproblem; the global planning of customer visits is generated by solving a master program. Confronted with the issue of symmetry in time, we used a state-space relaxation idea. Our algorithm provides solutions with reasonable deviation from optimality for large scale problems (260 customer sites, 60 time periods, 10 vehicles) coming from industry [73]. 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 [75].

Together with our partner company GAPSO from the associate team SAMBA, we worked on the equipment routing task scheduling problem [80] 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 [60] and exact algorithms [47]. A substantial research has been done on machine scheduling problems. A new compact MIP formulation was proposed for a large class of these problems [46]. An exact decomposition algorithm was developed for the NP-hard maximizing the weighted number of late jobs problem on a single machine [82]. A dominant class of schedules for malleable parallel jobs was discovered in the NP-hard problem to minimize the total weighted completion time [84]. We proved that a special case of the scheduling problem at cross docking terminals to minimize the storage cost is polynomially solvable [85], [83].

Another application area in which we have successfully developed MIP approaches is in the area of tactical production and supply chain planning. In [45], we proposed a simple heuristic for challenging multi-echelon problems that makes effective use of a standard MIP solver. [44] 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 [48] provide demonstrably stronger formulations for some problem classes than any previously proposed.

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 [55], [54], 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 [50]. We considered train timetabling problems and their re-optimization after a perturbation in the network [57], [56]. 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. 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.

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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 methodologies to address them. Most of our applications involve contracts with industrial partners, e.g. in reliability, although we also have several more academic collaborations, e.g. genomics, genetics and neuroimaging.

## 4.2. Curves classification

The field of classification for complex data as curves, functions, spectra and time series is important. Standard data analysis questions are being revisited to define new strategies that take the functional nature of the data into account. Functional data analysis addresses a variety of applied problems, including longitudinal studies, analysis of fMRI data and spectral calibration.

We are focusing on unsupervised classification. In addition to standard questions as the choice of the number of clusters, the norm for measuring the distance between two observations, and the vectors for representing clusters, we must also address a major computational problem. The functional nature of the data needs to be design efficient anytime algorithms.

## 4.3. Computer Experiments and Reliability

Since several years, SELECT has collaborations with EDF-DER *Maintenance des Risques Industriels* group. An important theme concerns 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 an high-technology group (Aerospace propulsion, Aircraft equipment, Defense Security, Communications).

Moreover, a collaboration has started with Dassault Aviation on modal analysis of mechanical structures, which aims at identifying the vibration behavior of structures under dynamic excitations. From algorithmic view point, modal analysis amounts to estimation in parametric models on the basis of measured excitations and structural responses data. As it appears from literature and existing implementations, the model selection problem attached to this estimation is currently treated by a rather heavy and very heuristic procedure. The model selection via penalisation tools are intended to be tested on this model selection problem.

## 4.4. Neuroimaging

Since 2007 SELECT participates to a working group with team Neurospin (CEA-INSERM-Inria) on Classification, Statistics and fMRI (functional Magnetic Resonance Imaging) analysis. In this framework two theses have been co-supervised by SELECT and Neurospin researchers (Merlin Keller 2006-2009 and Vincent Michel 2007-2010). The aim of this research is to determine which parts of the brain are activated by different types of stimuli. A model selection approach is useful to avoid "false-positive" detections.



## 4.5. Analysis of genomic data

Since many years 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 started a thesis cosupervised 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.

## 4.6. Environment

A study has been achieved by Jean-Michel Poggi, Michel Misiti, Yves Misiti and Bruno Portier (INSA de Rouen), in the context of a collaboration between AirNormand, Orsay University and INSA of Rouen. Two methods for spatial outlier detection have been considered: one based on the nearest neighbours weighted median and one based on kriging increments instead of more traditional pseudo-innovations. The two methods are applied to the PM10 monitoring network in Normandie (France) and are fully implemented in the Measurements Quality Control process.

## 4.7. Analysis spectroscopic imaging of ancient materials

Ancient materials, encountered in archaeology, paleontology and cultural heritage, are often complex, heterogeneous and poorly characterised before their physico-chemical analysis. A technique of choice to gather as much physico-chemical information as possible is spectro-microscopy or spectral imaging where a full spectra, made of more than 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 it requires the combination of an «image» approach with «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 dataset. This technic enablesx the simultaneous accounting for spatial and spectral information while producing statistically sound information on morphological and physico-chemical aspects of the studied samples.

## SequeL Project-Team

# 4. Application Domains

## 4.1. In Short

SEQUEL aims at solving problems of prediction, as well as problems of optimal and adaptive control. As such, the application domains are very numerous.

The application domains have been organized as follows:

- adaptive control,
- signal processing and functional prediction,
- medical applications,
- web mining,
- computer games.

## 4.2. Adaptive Control

Adaptive control is an important application of the research being done in SEQUEL. Reinforcement learning (RL) precisely aims at controlling the behavior of systems and may be used in situations with more or less information available. Of course, the more information, the better, in which case methods of (approximate) dynamic programming may be used [40]. But, reinforcement learning may also handle situations where the dynamics of the system is unknown, situations where the system is partially observable, and non stationary situations. Indeed, in these cases, the behavior is learned by interacting with the environment and thus naturally adapts to the changes of the environment. Furthermore, the adaptive system may also take advantage of expert knowledge when available.

Clearly, the spectrum of potential applications is very wide: as far as an agent (a human, a robot, a virtual agent) has to take a decision, in particular in cases where he lacks some information to take the decision, this enters the scope of our activities. To exemplify the potential applications, let us cite:

- game softwares: in the 1990's, RL has been the basis of a very successful Backgammon program, TD-Gammon [46] that learned to play at an expert level by basically playing a very large amount of games against itself. Today, various games are studied with RL techniques.
- many optimization problems that are closely related to operation research, but taking into account the uncertainty, and the stochasticity of the environment: see the job-shop scheduling, or the cellular phone frequency allocation problems, resource allocation in general [40]
- we can also foresee that some progress may be made by using RL to design adaptive conversational agents, or system-level as well as application-level operating systems that adapt to their users habits.

More generally, these ideas fall into what adaptive control may bring to human beings, in making their life simpler, by being embedded in an environment that is made to help them, an idea phrased as "ambient intelligence".

- The sensor management problem consists in determining the best way to task several sensors when each sensor has many modes and search patterns. In the detection/tracking applications, the tasks assigned to a sensor management system are for instance:
  - detect targets,
  - track the targets in the case of a moving target and/or a smart target (a smart target can change its behavior when it detects that it is under analysis),
  - combine all the detections in order to track each moving target,
  - dynamically allocate the sensors in order to achieve the previous three tasks in an optimal way. The allocation of sensors, and their modes, thus defines the action space of the underlying Markov decision problem.

In the more general situation, some sensors may be localized at the same place while others are dispatched over a given volume. Tasking a sensor may include, at each moment, such choices as where to point and/or what mode to use. Tasking a group of sensors includes the tasking of each individual sensor but also the choice of collaborating sensors subgroups. Of course, the sensor management problem is related to an objective. In general, sensors must balance complex trade-offs between achieving mission goals such as detecting new targets, tracking existing targets, and identifying existing targets. The word “target” is used here in its most general meaning, and the potential applications are not restricted to military applications. Whatever the underlying application, the sensor management problem consists in choosing at each time an action within the set of available actions.

- sequential decision processes are also very well-known in economy. They may be used as a decision aid tool, to help in the design of social helps, or the implementation of plants (see [44], [43] for such applications).

### 4.3. Signal Processing

Applications of sequential learning in the field of signal processing are also very numerous. A signal is naturally sequential as it flows. It usually comes from the recording of the output of sensors but the recording of any sequence of numbers may be considered as a signal like the stock-exchange rates evolution with respect to time and/or place, the number of consumers at a mall entrance or the number of connections to a web site. Signal processing has several objectives: predict, estimate, remove noise, characterize or classify. The signal is often considered as sequential: we want to predict, estimate or classify a value (or a feature) at time  $t$  knowing the past values of the parameter of interest or past values of data related to this parameter. This is typically the case in estimation processes arising in dynamical systems.

Signals may be processed in several ways. One of the best-known way is the time-frequency analysis in which the frequencies of each signal are analyzed with respect to time. This concept has been generalized to the time-scale analysis obtained by a wavelet transform. Both analysis are based on the projection of the original signal onto a well-chosen function basis. Signal processing is also closely related to the probability field as the uncertainty inherent to many signals leads to consider them as stochastic processes: the Bayesian framework is actually one of the main frameworks within which signals are processed for many purposes. It is worth noting that Bayesian analysis can be used jointly with a time-frequency or a wavelet analysis. However, alternatives like belief functions came up these last years. Belief functions were introduced by Demspter few decades ago and have been successfully used in the few past years in fields where probability had, during many years, no alternatives like in classification. Belief functions can be viewed as a generalization of probabilities which can capture both imprecision and uncertainty. Belief functions are also closely related to data fusion.

### 4.4. Medical Applications

One of the initial motivations of the multi-arm bandit theory stems from clinical trials when one researches the effects of different treatments while maximizing the improvement of the patients' health states.

Medical health-care and in particular patient-management is up today one of the most important applications of the sequential decision making. This is because the treatment of the more complex health problems is typically sequential: A physician repeatedly observes the current state of the patient and makes the decision in order to improve the health condition as measured for example by *qualys* (quality adjusted life years).

Moreover, machine learning methods may be used for at least two means in neuroscience:

1. as in any other (experimental) scientific domain, the machine learning methods relying heavily on statistics, they may be used to analyse experimental data,
2. dealing with induction learning, that is the ability to generalize from facts which is an ability that is considered to be one of the basic components of “intelligence”, machine learning may be considered as a model of learning in living beings. In particular, the temporal difference methods for reinforcement learning have strong ties with various concepts of psychology (Thorndike's law of effect, and the Rescorla-Wagner law to name the two most well-known).

## 4.5. Web Mining

We work on the news/ad recommendation. These online learning algorithms reached a critical importance over the last few years due to these major applications. After designing a new algorithm, it is critical to be able to evaluate it without having to plug it into the real application in order to protect user experiences or/and the company's revenue. To do this, people used to build simulators of user behaviors and try to achieve good performances against it. However designing such a simulator is probably much more difficult than designing the algorithm itself! An other common way to evaluate is to not consider the exploration/exploitation dilemma (also known as "Cold Start" for recommender systems). Lately data-driven methods have been developed. We are working on building automatic replay methodology with some theoretical guarantees. This work also exhibits strong link with the choice of the number of contexts to use with recommender systems wrt your audience.

An other point is that web sites must forecast Web page views in order to plan computer resource allocation and estimate upcoming revenue and advertising growth. In this work, we focus on extracting trends and seasonal patterns from page view series. We investigate Holt-Winters/ARIMA like procedures and some regularized models for making short-term prediction (3-6 weeks) wrt to logged data of several big media websites. We work on some news event related webpages and we feel that kind of time series deserves a particular attention. Self-similarity is found to exist at multiple time scales of network traffic, and can be exploited for prediction. In particular, it is found that Web page views exhibit strong impulsive changes occasionally. The impulses cause large prediction errors long after their occurrences and can sometimes be predicted (*e.g.*, elections, sport events, editorial changes, holidays) in order to improve accuracies. It also seems that some promising model could arise from using global trends shift in the population.

## 4.6. Games

The problem of artificial intelligence in games consists in choosing actions of players in order to produce artificial opponents. Most games can be formalized as Markov decision problems, so they can be approached with reinforcement learning.

In particular, SEQUEL was a pioneer of Monte Carlo Tree Search, a technique that obtained spectacular successes in the game of Go. Other application domains include the game of poker and the Japanese card game of hanafuda.

## **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.

#### **4.2. Natural Language Processing**

This year, our research has focused on new application domains within natural language processing (NLP), with our first two publications in leading conferences in NLP. We have worked on large-scale semantic role labelling (E. Grave, F. Bach, G. Obozinski), where we use syntactic dependency trees and learned representations from large corpora (e.g., 14.7 millions sentences, 310 millions tokens). We also extended our original work on structured sparsity to language models (F. Bach, A. Nelakanti, in collaboration with Xerox), in order to predict a word given *all* previous words, with a potentially infinite feature space organized with structured regularization.

## 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);
  - Tenths of years, for investments.

Nice challenges also include:

- Spatial distribution of problems; due to capacity limits we cannot consider a power grid like Europe + North Africa as a single “production = demand” constraint; with extra connections we can balance excess production by renewables for remote areas, although to a limited extent.
- Other uncertainties, which might be modeled by adversarial or stochastic frameworks (e.g., technological breakthroughs, decisions about ecological penalization).

We have several related projects (Citines, a European (FP7) project; in the near future we should start the Post project (ADEME); IOMCA, a ANR project), and POST, a ADEME project about investments in power systems. We have a collaboration with the SME Artelys, that works on optimization in general, and on energy management in particular.

**Technical challenges:** Our work focuses on the combination of reinforcement learning tools, with their anytime behavior and asymptotic guarantees, with existing fast approximate algorithms; see 6.2 . 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.

**Related Activities:**

- We are in the process of creating a Franco-Taiwanese company (maybe a Taiwanese company using French software) for energy optimization in Taiwan.
- We have a joint team with Taiwan, namely the Indema associate team (see Section 8.4.1.1 ).
- We have an I-lab in progress with Artelys (see Section 5.1 ) in order to ensure the transfer of our work.
- We have organized various forums and meetings around Energy Management.

#### 4.2. Air Traffic Control

Air Traffic Control has been an application field of Marc Schoenauer’s work in the late 90s (PhD theses of F. Médioni in 1998 and S. Oussedik in 2000). It was revived recently with Gaëtan Marceau-Caron’s CIFRE PhD together with Thalès Air Systems (Areski Hadjaz) and Thalès TRT (Pierre Savéant), tackling the global optimization of the traffic in order to increase the capacity of the airspace without overloading the controllers. A new formulation of the problem, modeling the plane flows with Bayesian Networks, has been proposed to the Air Traffic Control community [48], [50]. The goal of the optimization is to minimize the cumulated delays of all flights, while maintaining a reasonable level of congestion in all sectors. These objectives are computed using Monte-Carlo simulations of the Bayesian network, and Evolutionary Algorithms are used to address the resulting stochastic multi-objective optimization problem [49].

## ALEA Project-Team

# 4. Application Domains

## 4.1. Application Domains

This short section is only concerned with the list of concrete application domains developed by our team project on Bayesian inference and unsupervised learning, nonlinear filtering and rare event analysis. Most of these application areas result from fruitful collaborations with other national institutes or industries.

Three application domains are directly related to evolutionary computing, particle filtering and Bayesian inference. They are currently investigated by our team project:

1. **Multi-object tracking.** Multi-object tracking deals with the task of estimating the states of a set of moving objects from a set of measurements obtained sequentially. These measurements may either arise from one of the targets or from clutter and the measurement-to-target association is generally unknown. This problem can then be recast as a dynamic clustering one where the clusters are the clutter and the different targets. The targets actually move in time, some targets may appear/disappear over time and the number of targets is generally unknown and time-varying. The ALEA team has been involved in the ANR project Propagation with DCNS, Thalés and Exavision.
2. **Finance.** The Team ALEA is interested in the design and analysis of new advanced particle methods for option pricing, partial observation problems, and sensitivity measures computation. An **international workshop** has been jointly organized by ALEA and **CMAF (Polytechnique)** on this topic in October 2012 (organizers: E. Gobet, P. Del Moral, P. Hu).
3. **Epidemiology.** Our team is interested in the development and analysis of particle mean field models for the calibration and uncertainty propagations in complex kinetic population models. The ALEA team is involved in an interdisciplinary exploratory research project with Laboratory Ecologie & Evolution, and co-organized an **international workshop** on this topic in 2011.

## ASPI Project-Team

### 4. Application Domains

#### 4.1. Localisation, navigation and tracking

See 5.11 .

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 [43], [37], 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 [42], [56], 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 5.3 , 5.6 , and 5.7 .

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 [50], 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 all the topics of team is a collaboration started in May 2010 with Thales Optronique on the subject of *optimization of the maintenance of a digital camera equipped with HUMS* (Health Unit Monitoring Systems). This subject is very interesting for us because it combines many aspects of our project. Classification tools will be used to select significant variables as the first step in the modeling of a digital camera. The model will then be analysed and estimated in order to optimize the maintenance.

A second example concerns the optimization of the maintenance date for an aluminum metallic structure subject to corrosion. It is a structure of strategic ballistic missile that is stored in a nuclear submarine missile launcher in peace-time and inspected with a given periodicity. The requirement for security on this structure is very strong. The mechanical stress exerted on the structure depends on its thickness. It is thus crucial to control the evolution of the thickness of the structure over time, and to intervene before the break.

A third example is the minimization of the acoustic signature of a submarine. The submarine has to chose its trajectory in order to minimize at each time step its observability by a surface ship following an unknown random trajectory.

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, Systemic Risk, Portfolio optimization, Risk modeling.

## REGULARITY Project-Team

### 4. Application Domains

#### 4.1. Uncertainties management

Our theoretical works are motivated by and find natural applications to real-world problems in a general frame generally referred to as uncertainty management, that we describe now.

Since a few decades, modeling has gained an increasing part in complex systems design in various fields of industry such as automobile, aeronautics, energy, etc. Industrial design involves several levels of modeling: from behavioural models in preliminary design to finite-elements models aiming at representing sharply physical phenomena. Nowadays, the fundamental challenge of numerical simulation is in designing physical systems while saving the experimentation steps.

As an example, at the early stage of conception in aeronautics, numerical simulation aims at exploring the design parameters space and setting the global variables such that target performances are satisfied. This iterative procedure needs fast multiphysical models. These simplified models are usually calibrated using high-fidelity models or experiments. At each of these levels, modeling requires control of uncertainties due to simplifications of models, numerical errors, data imprecisions, variability of surrounding conditions, etc.

One dilemma in the design by numerical simulation is that many crucial choices are made very early, and thus when uncertainties are maximum, and that these choices have a fundamental impact on the final performances.

Classically, coping with this variability is achieved through *model registration* by experimenting and adding fixed *margins* to the model response. In view of technical and economical performance, it appears judicious to replace these fixed margins by a rigorous analysis and control of risk. This may be achieved through a probabilistic approach to uncertainties, that provides decision criteria adapted to the management of unpredictability inherent to design issues.

From the particular case of aircraft design emerge several general aspects of management of uncertainties in simulation. Probabilistic decision criteria, that translate decision making into mathematical/probabilistic terms, require the following three steps to be considered [58]:

1. build a probabilistic description of the fluctuations of the model's parameters (*Quantification of uncertainty sources*),
2. deduce the implication of these distribution laws on the model's response (*Propagation of uncertainties*),
3. and determine the specific influence of each uncertainty source on the model's response variability (*Sensitivity Analysis*).

The previous analysis now constitutes the framework of a general study of uncertainties. It is used in industrial contexts where uncertainties can be represented by *random variables* (unknown temperature of an external surface, physical quantities of a given material, ... at a given *fixed time*). However, in order for the numerical models to describe with high fidelity a phenomenon, the relevant uncertainties must generally depend on time or space variables. Consequently, one has to tackle the following issues:

- *How to capture the distribution law of time (or space) dependent parameters, without directly accessible data?* The distribution of probability of the continuous time (or space) uncertainty sources must describe the links between variations at neighbor times (or points). The local and global regularity are important parameters of these laws, since it describes how the fluctuations at some time (or point) induce fluctuations at close times (or points). The continuous equations representing the studied phenomena should help *to propose models for the law of the random fields*. Let us notice that interactions between various levels of modeling might also be used to derive distributions of probability at the lowest one.

- The navigation between the various natures of models needs a kind of *metric* which could *mathematically describe the notion of granularity or fineness* of the models. Of course, the local regularity will not be totally absent of this mathematical definition.
- All the various levels of conception, preliminary design or high-fidelity modelling, require *registrations by experimentation* to reduce model errors. This *calibration* issue has been present in this frame since a long time, especially in a deterministic optimization context. The random modeling of uncertainty requires the definition of a systematic approach. The difficulty in this specific context is: statistical estimation with few data and estimation of a function with continuous variables using only discrete setting of values.

Moreover, a multi-physical context must be added to these questions. The complex system design is most often located at the interface between several disciplines. In that case, modeling relies on a coupling between several models for the various phenomena and design becomes a *multidisciplinary optimization* problem. In this uncertainty context, the real challenge turns robust optimization to manage technical and economical risks (risk for non-satisfaction of technical specifications, cost control).

We participate in the uncertainties community through several collaborative research projects. As explained above, we focus on essentially irregular phenomena, for which irregularity is a relevant quantity to capture the variability (e.g. certain biomedical signals, terrain modeling, financial data, etc.). These will be modeled through stochastic processes with prescribed regularity.

## 4.2. Biomedical Applications

### ECG analysis and modelling

ECG and signals derived from them are an important source of information in the detection of various pathologies, including *e.g.* congestive heart failure, arrhythmia and sleep apnea. The fact that the irregularity of ECG bears some information on the condition of the heart is well documented (see *e.g.* the web resource <http://www.physionet.org>). The regularity parameters that have been studied so far are mainly the box and regularization dimensions, the local Hölder exponent and the multifractal spectrum [61], [63]. These have been found to correlate well with certain pathologies in some situations. From a general point of view, we participate in this research area in two ways.

- First, we use refined regularity characterizations, such as the regularization dimension, 2-microlocal analysis and advanced multifractal spectra for a more precise analysis of ECG data. This requires in particular to test current estimation procedures and to develop new ones.
- Second, we build stochastic processes that mimic in a faithful way some features of the dynamics of ECG. For instance, the local regularity of RR intervals, estimated in a parametric way based on a modelling by an mBm, displays correlations with the amplitude of the signal, a feature that seems to have remained unobserved so far [3]. In other words, RR intervals behave as SRP. We believe that modeling in a simplified way some aspects of the interplay between the sympathetic and parasympathetic systems might lead to an SRP, and to explain both this self-regulating property and the reasons behind the observed multifractality of records. This will open the way to understanding how these properties evolve under abnormal behaviour.

### Pharmacodynamics and patient drug compliance

Poor adherence to treatment is a worldwide problem that threatens efficacy of therapy, particularly in the case of chronic diseases. Compliance to pharmacotherapy can range from 5% to 90%. This fact renders clinical tested therapies less effective in ambulatory settings. Increasing the effectiveness of adherence interventions has been placed by the World Health Organization at the top list of the most urgent needs for the health system. A large number of studies have appeared on this new topic in recent years [75], [74]. In collaboration with the pharmacy faculty of Montréal university, we consider the problem of compliance within the context of multiple dosing. Analysis of multiple dosing drug concentrations, with common deterministic models, is usually based on patient full compliance assumption, *i.e.*, drugs are administered at a fixed dosage. However, the drug concentration-time curve is often influenced by the random drug input generated by patient poor

adherence behaviour, inducing erratic therapeutic outcomes. Following work already started in Montréal [67], [68], we consider stochastic processes induced by taking into account the random drug intake induced by various compliance patterns. Such studies have been made possible by technological progress, such as the “medication event monitoring system”, which allows to obtain data describing the behaviour of patients.

We use different approaches to study this problem: statistical methods where enough data are available, model-based ones in presence of qualitative description of the patient behaviour. In this latter case, piecewise deterministic Markov processes (PDP) seem a promising path. PDP are non-diffusion processes whose evolution follows a deterministic trajectory governed by a flow between random time instants, where it undergoes a jump according to some probability measure [55]. There is a well-developed theory for PDP, which studies stochastic properties such as extended generator, Dynkin formula, long time behaviour. It is easy to cast a simplified model of non-compliance in terms of PDP. This has allowed us already to obtain certain properties of interest of the random concentration of drug [37]. In the simplest case of a Poisson distribution, we have obtained rather precise results that also point to a surprising connection with infinite Bernoulli convolutions [37], [13], [12]. Statistical aspects remain to be investigated in the general case.

## 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 Finance, Neuroscience and Biology, Fluid Mechanics and Meteorology, Chemical Kinetics, Diffusions in random media, Transverse problems, Software and Numerical experiments.

**Finance** For a long time now TOSCA has collaborated with researchers and practitioners in various financial institutions and insurance companies. We are particularly interested in calibration problems, risk analysis (especially model risk analysis), optimal portfolio management, Monte Carlo methods for option pricing and risk analysis, asset and liabilities management. We also work on the partial differential equations related to financial issues, for example the stochastic control Hamilton–Jacobi–Bellman equations. We study existence, uniqueness, qualitative properties and appropriate deterministic or probabilistic numerical methods. At the moment we pay special attention to the financial consequences induced by modelling errors and calibration errors on hedging strategies and portfolio management strategies.

**Neuroscience and Biology** The interest of TOSCA in biology is developing in three main directions: neuroscience, molecular dynamics and population dynamics. In neuroscience, stochastic methods are developed to analyze stochastic resonance effects, to solve inverse problems and to investigate mean-field/McKean-Vlasov equations. For example, we are studying probabilistic interpretations and Monte Carlo methods for divergence form second-order differential operators with discontinuous coefficients, motivated by the 3D MEG inverse problem. Our research in molecular dynamics focuses on the development of Monte Carlo methods for the Poisson-Boltzmann equation which also involves a divergence form operator, and of original algorithms to construct improved simulation techniques for protein folding or interaction. Finally, our interest in population dynamics comes from ecology, evolution and genetics. For example, we are studying the emergence of diversity through the phenomenon of evolutionary branching in adaptive dynamics. Some collaborations in biostatistics on cancer problems are also being initiated.

**Fluid Mechanics and Meteorology** In Fluid Mechanics we develop probabilistic methods to solve vanishing viscosity problems and to study the behavior of complex flows at the boundary, and their interaction with the boundary. We elaborate and analyze stochastic particle algorithms. Our studies concern the convergence analysis of these methods on theoretical test cases and the design of original schemes for applicative cases. A first example concerns the micro-macro model of polymeric fluids (the FENE model). A second example concerns stochastic Lagrangian modelling of turbulent flows. We are particularly motivated by the meteorological downscaling, and by the computation of characteristic properties of the local wind activity in areas where windmills are built. Our goal is to estimate local potential resources which are subject to meteorological variability (randomness) by developing a stochastic downscaling methodology, that is able to refine wind prevision at large scale, and to compute management strategies of wind resources.

**Chemical Kinetics** The TOSCA team is studying coagulation and fragmentation models, that have numerous areas of applications (polymerization, aerosols, cement industry, copper industry, population dynamics...). Our current motivation comes from the industrial copper crushers in Chile. We aim to model and calibrate the process of fragmentation of brass particles of copper in industrial crushers, in order to improve their efficiency at a low cost.

**Diffusions in random media** A *random medium* is a material with a lot of heterogeneity which can be described only statistically. Typical examples are fissured porous media within rocks of different types, turbulent fluids or unknown or deficient materials in which polymers evolve or waves

propagate. For the last few years, the TOSCA team has been collaborating with the Geophysics community on problems related to underground diffusions, especially those which concern waste transport or oil extraction. We are extending our previous results on the simulation of diffusion processes generated by divergence form operators with discontinuous coefficients. Such an operator appears for example in the Darcy law for the behavior of a fluid in a porous media. We are also developing another class of Monte Carlo methods to simulate diffusion phenomena in discontinuous media.

**Transverse problems** Several of the topics of interest of TOSCA do not only concern a single area of application. This is the case in particular for long time simulation methods of nonlinear McKean-Vlasov PDEs, the problem of simulation of multivalued models, variance reduction techniques or stochastic partial differential equations. For example, multivalued processes have applications in random mechanics or neuroscience, and variance reduction techniques have applications in any situation where Monte Carlo methods are applicable.

**Software, numerical experiments** TOSCA is interested in designing algorithms of resolution of specific equations in accordance with the needs of practitioners. We benefit from our strong experience of the programming of probabilistic algorithms of various architectures including intensive computation architectures. In particular, our activity will concern the development of grid computing techniques to solve large dimensional problems in Finance. We are also interested in intensively comparing various Monte Carlo methods for PDEs and in the development of open source libraries for our numerical methods in Fluid Mechanics, MEG or Chemical Kinetics.