RESEARCH CENTER

FIELD
Applied Mathematics, Computation and Simulation

Activity Report 2013

Section New Results

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CAD Team

5. New Results

5.1. Geometry

5.1.1. From CAD to Engineering: Computing FEM on curved surfaces

Participants: Jean-Claude Paul, Kan-Le Shi, Yu-Shen Liu, Jin-San Cheng, Cheng-Lei Yang, Bruno Durand, Jun-Hai Yong.

In cooperation with Bruno Lévy (Inria)

The cooperation with EADS, based on our new B-Spline surface formulation, was very promising, for complex shape modelling. Our surfaces are very efficient in term of precision. Moreover, they avoid the control point explosion of NURBS surfaces. We propose our work in two directions: 1) to Improve the Modelling process for the user (it is a strategic point of the success of our new mathematical surface); 2) to take profit of the control points way of our surface to compute numerical simulation on this surface directly. In industry, Geometry design and Engineering employ a sequence of tools that are generally not well matched to each other. For example, the output of a computer aided geometric design system is typically not suitable as direct input for a finite-element modeler. This is usually addressed through intermediate tools such as mesh generators. Unfortunately, these are notoriously lacking in robustness. Even once a geometric model has been successfully meshed, the output of a finite-element simulation cannot be directly applied to the original geometric model, since there is no straightforward mapping back to the original design degrees of freedom. Additionally there is a need for a trade-off between the speed of analysis and the fidelity of the results. In the early stages of design, quick results are necessary, but approximate results are acceptable. In the later stages, highly precise results are required, and longer computation times are tolerated. Worse, different underlying models are required for each level of refinement. These difficulties make the design process cumbersome and inhibit rapid iteration over design alternatives. We plan to use FEA on Knot vectors surfaces directly (i.e. use the same function basis for the Geometric Modeling and the Numerical Simulation Process. We will apply this approach to fluids analysis: turbulence modeling (fluid-structure interaction). We think that our surface functions exhibiting higher-order continuity are an ideal candidate for approximating such flows. From the practical point of view, the main objectives of the study are to evaluate, in the scope of this application, the efficiency of such approach in term of simulation accuracy, simulation time and computational convergence. We also aim to evaluation how such approach deals with simulation accuracy/convergence according to CAD definition (quality/size of patches used to define the 3D shape).

5.1.2. From CAD to Manufacturing: Robustness tolerance and error control

Participants: Jun-Hai Yong, Yu-Shen Liu, Clara Issandou, Hai-Chuan Song, Lu Yang, Kang-Lai Qian, Jean-Claude Paul.

In cooperation with Dr. Nabil Anwer – ENS Cachan and the Tsinghua PLM Center (supported by Dassault System). Dr. Yi-Jun Yang (Shandong University), Dr. Xiao-Diao Chen (Zhejiang University)

Based on our theoretical contribution in Differential Geometry, especially about our ϵ-Geometry Continuity and our new geometric operators we proposed several elegant solutions to the most important challenges in Computer Aided Design (see Lees A Piegl. "Ten challenges in Computer-Aided-Design". Jal of CAD 2005. 37 (4): 461-470): robustness, tolerances, error control. During CAD processes one uses a myriad of tolerances, many of which are directly related to the actual manufacturing process. Some interesting questions here include: What are the most relevant machining tolerances? How to set the army of computational tolerances, e.g. those of systems of equations, to guarantee machining within the required accuracy? How tolerances in different spaces, e.g. in model space and in parameter space, are related. Numerical instabilities also account for the majority of computational errors in commercial CAD systems. The problems related to robustness

haunt every programmer who has ever worked on commercial systems. Fixing numerical bugs can be very frustrating, and often times results in patching up the code simply because no solution exists to remedy the problem. We first plan for assisting the designer when specifying the functional tolerances of a single part included in a mechanism, without any required complex function analysis. The mechanism assembly is first described through a positioning table formalism. In order to create datum reference frames and to respect assembly requirements, an ISO based 3D tolerancing scheme will be proposed, thanks to a set of rules based on geometric patterns and TTRS (Technologically and Topologically Related Surfaces). Since it remains impossible to determine tolerance chains automatically, the designer must impose links between the frames. We want to develop proposes ISO based tolerance specifications to help ensure compliance with the designer's intentions, saving on time and eliminating errors.

5.2. Computer Graphics (2010-2013)

5.2.1. Inverse Procedural Modeling of Facade Layouts

Participants: Weiming Dong, Bin Wang, Dong-Ming Yan, Hua-Liang Xie, Jean-Claude Paul.

We want to address the following open research problem: How can we generate a deterministic shape grammar that explains a given facade layout? An approximate dynamic programming framework will tackle this problem. The proposed solution contributes to the compression of urban models, architectural analysis, and the generation of shape grammars for large-scale urban modeling. As a major contribution of this work we want to formulate the inverse procedural modeling problem for facade layouts as a smallest grammar problem. We also want to propose an automatic algorithm to derive a shape grammar for a given facade layout. In this work, we will assume segmented and labeled facade layouts as input and do not derive the shape grammars directly from photographs. The joint optimization of segmentation and grammar extraction remains an aspirational goal for this work.

5.2.2. Architecture Design

Participants: Jean-Claude Paul, Bin Wang, Weiming Dong, Lin Li, Yan Kong, Yong Zhang, Fan Tang, Fuzhang Wu, Cui-Gong Wang.

In cooperation with UC Berkeley - Department of Architecture

We want to propose a method for automated generation of architectural models for computer graphics applications. Our focus is not only on the building layout: the internal organization of spaces within the building, but also the Architectural composition of volumes, roofs and facades. We focus on the generation of various types of buildings: residences, schools, museums, hospitals, civic enters, office buildings. Our work builds on grammar-based procedural modeling, inverse procedural modeling and composition rules, especially symmetry and scaling, and interactivity. Moreover, we consider the architecture design process as an iterative trial-and-error process that requires significant expertise and learning by doing.

CALVI Project-Team

6. New Results

6.1. Software development

6.1.1. New methods in Selalib

The Selalib library has seen important developments during the year 2013 as we move towards a release in 2014. Several existing modules were improved in terms of their interfaces or implementations, while many other modules were added. Notably, we have improved our interaction with external software (Pigasus, developed by Dr. Ahmed Ratnani) capable of producing NURBS-based coordinate transformations and introduced a general elliptic PDE solver based on finite elements and arbitrary degree splines that can be used as a field solver in domains deformed by an arbitrary coordinate transformation. Preliminary results of these developments have been published [2]. In addition, we have included new abstractions to facilitate the development of parallel codes using domain decomposition methods. Modules like these have been already used in some of the multiple pre-packaged simulations also included during this period. For instance, it allows us to implement a new Vlasov-Poisson solver by the Eulerian reduced approach, with applications to four-dimensional Landau-Damping. The latest simulations also use newly developed interfaces related with the semi-lagrangian methodology, such as generic interfaces for advections and calculation of characteristics. At the end of 2013 virtually all conceivable abstractions related with the semi-lagrangian methodology have a natural place to live within the library.

Many new and classical methods and models have been cleanly incorporated into our software Selalib:

- Vlasov-Poisson solver by the Eulerian reduced approach. Application to 4D Landau-Damping.
- cartesian semi-Lagrangian 2D guiding center sequential simulation tested on periodic Kelvin Helmholtz instability
- polar semi-Lagrangian 2D guiding center sequential simulation tested on diocotron instability
- general curvilinear semi-Lagrangian 2D guiding center sequential simulation; first results, still in progress
- cartesian semi-Lagrangian 2D Vlasov-Poisson parallel simulation with high order splitting tested on Landau damping, bump on tail, two stream instability and beam
- cartesian semi-Lagrangian 2D Vlasov-Poisson sequential simulation without splitting tested on beam
- cartesian semi-Lagrangian 4D Vlasov-Poisson parallel simulation on cartesian grid with high order splitting tested on Landau-Damping
- polar semi-Lagrangian 4D drift kinetic parallel simulation tested on a simple ITG instability
- general curvilinear semi-Lagrangian 4D drift kinetic parallel simulation (in development)

6.1.2. New developments in CLAC

CLAC is a generic DG solver for hyperbolic conservation laws. It is optimized for running efficiently on GPU clusters. We have reorganized the software conception in order to accelerate the computations. A first point is to group the finite-elements into uniform zones in order to get optimized kernels for SIMD architectures. A second point is to manage efficiently the data transfers between the zone. An important last point is to consider a non blocking parallel task management. This is achieved through a coupling between the event mechanisms of OpenCL and MPI. Some ideas and results are presented in [44]. In addition to these developments, we have started to test some parallel programming approaches in order to achieve good efficiency on multicore processors. These ideas have been tested on fluid models [27] and the MHD model [47]. They are very efficient and will be incorparated into CLAC later on.

[2] A. Back, E. Chacon-Golcher, V. Grandgirard, A. Ratnani, E. Sonnendrücker, A 4D semi-Lagrangian Vlasov solver based on an arbitrary curvilinear grid in physical space, poster at Vlasovia, 25-28 November 2013, Nancy

6.2. Mathematical analysis of kinetic models

Participants: N. Besse, M. Bostan.

Contribution [13] concerns a one-dimensional version of the Vlasov equation dubbed the Vlasov-Dirac-Benney equation (in short V-D-B) where the self interacting potential is replaced by a Dirac mass. Emphasis is put on the relations between the linearized version, the full nonlinear problem and equations of fluids. In particular the connection with the so-called Benney equation leads to new stability results. Eventually the V-D-B appears to be at the cross road of several problems of mathematical physics which have as far as stability is concerned very similar properties.

The subject matter of paper [3] concerns anisotropic diffusion equations: we consider heat equations whose diffusion matrices have disparate eigenvalues. We determine first and second order approximations, we study their well-posedness and then, we establish convergence results. The analysis relies on averaging techniques, which have been used previously for studying transport equations whose advection fields have disparate components.

In [4] we perform an asymptotic analysis of general particle systems arising in collective behavior in the limit of large self-propulsion and friction forces. These asymptotics impose a fixed speed in the limit, and thus a reduction of the dynamics to a sphere in the velocity variables. The limit models are obtained by averaging with respect to the fast dynamics. We can include all typical effects in the applications: short-range repulsion, long-range attraction, and alignment. For instance, we can rigorously show that the Cucker-Smale model is reduced to the Vicsek model without noise in this asymptotic limit. Finally, a formal expansion based on the reduced dynamics allows us to treat the case of diffusion. This technique follows closely the gyroaverage method used when studying the magnetic confinement of charged particles. The main new mathematical difficulty is to deal with measure solutions in this expansion procedure.

6.2.1. Gyrokinetic approximation

Participants: E. Frénod, M. Lutz.

Considering a Hamiltonian Dynamical System describing the motion of charged particle in a Tokamak or a Stellarator, we build in [42] a change of coordinates to reduce its dimension. This change of coordinates is in fact an intricate succession of mappings that are built using Hyperbolic Partial Differential Equations, Differential Geometry, Hamiltonian Dynamical System Theory and Symplectic Geometry, Lie Transforms and a new tool which is here introduced : Partial Lie Sums.

6.3. Development of semi-Lagrangian methods

Participants: N. Crouseilles, P. Glanc, A. Hamiaz, S. Hirstoaga, M. Mehrenberger, J. Petri, E. Sonnendrücker, C. Steiner.

The development of numerical methods - here semi-Lagrangian schemes for plasma physic applications- is continued and strengthened in the context of the on-going library Selalib. We intend to improve the robustness of the numerical tools in order to be prepared for future more realistic test problems.

6.3.1. Vlasov-Poisson simulations on cartesian grids

We have developed a 1D x 1D Vlasov-Poisson solver on GPU using optimized FFT of CUDA and applied it on KEEN waves test case, which needs a fine resolution in velocity [46]. An efficiency of 100 Gflops on 4096x4096 grid is obtained while using single precision, and about 30 GFlops on a 2048x3048 grid using double precision. The approach is valid: implementation effort is reduced, because we rely on external optimizations and the speed-up is quite impressive (only 1 or 2 GFlops were obtained using CPU). We emphasize that FFT is used for the implementation but not (necessarily) for the numerical method. Classical methods like splines or arbitrary high order odd Lagrange interpolation are used, as they can be fitted in

[3] M. Bostan, Strongly anisotropic diffusion problems; asymptotic analysis, in *J. Differential Equations*, vol. 256 pp. 1043-1092 (2013)

[4] M. Bostan, J.-A. Carrillo, Asymptotic fixed speed reduced dynamics for kinetic equations in swarming, *Math. Models Methods Appl. Sci.*, Vol.23, No. 13 pp. 2353-2393 (2013)

this framework. In order to reduce mass conservation issues while using single precision, a delta-f method is validated. The limitation is here the grid size; we were not able to run the code for bigger sizes. We then developed other strategies based on non uniform grids in velocity with cubic splines and two grid strategies [5] and with the semi-Lagrangian discontinuous Galerkin (SLDG) scheme [6]. Integration of the code in Selalib with upgraded interface to deal with non uniform grids has been thought but remains to be done. Thanks to the MPI Parallelization of the Selalib code, we should be able to run the code for more interesting physical parameters, in particular, when the drive amplitude goes to zero, which leads to even more localized delta-f function in velocity.

Considering the SLDG scheme, we were able to prove a super convergence property in the case of constant linear advection [48].

6.3.2. Guiding-center based simulations on polar grids

We continue our work on polar grids, which are intermediate, between cartesian and general curvilinear grids. We have revisited a diocotron simulation previously done with the PIC method [75] by using a (classical) semi-Lagrangian approach. A detailed study of boundary conditions, energy and mass conservation as well as linear growth rates is performed and validated with teh code [33]. We then have extended the code to a first drift kinetic simulation [7] using at first the classical cubic splines method and then a new 2D conservative method, called CSL2D (conservative semi-Lagrangian 2D), based on mesh intersections and displacement of volumes [11]. For the latter method to work, we had to take care of the Jacobian and we used a delta-f method, in order to treat more easily non zero boundary conditions. We have benefitted from previous experience on the FSL2D (forward semi-Lagrangian) method. Again, the integration in Selalib is under development. Linear growth rate is here validated, by solving numerically the dispersion relation using recent results of [21].

6.3.3. Guiding-center simulations on general curvilinear grids

In order to deal with more complex geometries or to consider field aligned coordinates, we work on generalizing existing methods for curvilinear grids. Guiding center simulations have been successfully performed with the classical cubic splines method and a finite element solver for the Poisson equation developed by A. Back [32]. Further works concern integration in Selalib, in a more modular way. This should help the comparison with other methods as for example the recent CSL2D method [11] but also the previous CSL1D method [5].

6.4. Development of reduced Eulerian methods

Participants: E. Chacon Golcher, P. Helluy, L. Navoret, N. Pham.

6.4.1. Eulerian methods in the physical phase-space

Kinetic plasmas computer simulations are very intensive, because of the gyrokinetic turbulence. In some situations, it is possible to make assumptions on the shape of the distribution function that simplify the model. We obtain in this way a family of fluid or reduced models.If the distribution function has a Maxwellian shape (strong collisions), we obtain the MagnetoHydroDynamic (MHD) model. Even without collisions, the plasma may still relax to an equilibrium state over sufficiently long time scales (Landau damping effect). This indicates that the approximation of the distribution function could require fewer data while still achieving a good representation, even in the collisionless regime. In what follows we call this the “reduced model” approach. A reduced model is a model where the explicit dependence on the velocity variable is suppressed. In a more mathematical way, we consider that in some regions of the plasma, it is possible to exhibit a (preferably small) set of parameters α that allows us to describe the main properties of the plasma with a generalized

[5] M. Mehrenberger, N. Crouseilles, E. Sonnendrücker, B. Afeyan High-Order Numerical Methods for KEEN Wave Vlasov-Poisson Simulations, Poster at PPPS, 16-21 June 2013, San Francisco

[6] C. Steiner, M. Mehrenberger, A semi-Lagrangian discontinuous Galerkin scheme for Vlasov-Poisson equation, poster at Vlasovia, 25-28 November 2013, Nancy

[7] N. Crouseilles, P. Glanc, S. Hirstoaga, E. Madaule, M. Mehrenberger, J. Pétri, Semi-Lagrangian simulations on polar grids: from diocotron instability to ITG turbulence, poster at Vlasovia, 25-28 November 2013, Nancy

"Maxwellian" M . Then $f(x,v,t) = M(\alpha(x,t),v)$. In this case it is sufficient to solve for $\alpha(x,t)$. Generally, the vector α is solution of a first order hyperbolic system.

Several approaches are possible that we have started to study theoretically and numerically: waterbag approximations, velocity space transforms, etc.

It is also possible to construct in this way intermediate models between the kinetic and the fluid models by truncating the velocity expansion. The unknowns α of the problem become the coefficients of the expansion, which depend only on space and time. They obey a first order hyperbolic PDE system. And then it is possible to capitalize on the large theoretical and numerical machinery developed for such PDEs.

A first step is to develop the one-dimensional models in order to test several numerical methods. The chosen approach is the high order Discontinuous Galerkin (DG) family of methods for solving the hyperbolic system. We compare the reduced Eulerian model with semi-Lagrangian or PIC methods on classical test cases: Landau damping, two-stream instability [28].

6.4.2. *Eulerian method in the Fourier transformed phase-space*

An experiment made in the 60's [8] exhibits in a spectacular way the reversible nature of the Vlasov equations. When two perturbations are applied to a plasma at different times, at first the plasma seems to damp and reach an equilibrium. But the information of the perturbations is still here and "hidden" in the high frequency microscopic oscillations of the distribution function. At a later time a resonance occurs and the plasma produces an echo. The time at which the echo occurs can be computed (see Villani[9], page 74). The fine mathematical study of this phenomenon allowed C. Villani and C. Mouhot to prove their famous result on the rigorous nonlinear Landau damping[10].

More practically, this experiment and its theoretical framework show that it is interesting to represent the distribution function by an truncated expansion on an orthonormal basis of oscillating functions in the velocity variables. This representation allows a better control of the energy transfer between the low frequencies and the high frequencies in the velocity direction, and thus provides more relevant numerical methods. This kind of approach is studied for instance by Eliasson [11].

We have started to study such kind of approaches in [43]. An interesting point is that the truncated reduced model is also an hyperbolic system in the space direction only. This allows the classical methods for hyperbolic systems to be reused.

6.5. Two-Scale numerical methods

Participant: E. Frénod.

In note [39] a classification of Homogenization-Based Numerical Methods and (in particular) of Numerical Methods that are based on the Two-Scale Convergence is done. In this classification stand: Direct Homogenization-Based Numerical Methods, H-Measure-Based Numerical Methods, Two-Scale Numerical Methods and TSAPS (Two-Scale Asymptotic Preserving Schemes).

In [34] we develop and we explain the two-scale convergence in the covariant formalism, i.e. using differential forms on a Riemannian manifold. For that purpose, we consider two manifolds M and Y, the first one contains the positions and the second one the oscillations. We establish some convergence results working on geodesics on a manifold. Then, we apply this framework on examples.

6.6. Spline Discrete Differential Forms and applications

Participant: E. Sonnendrücker.

[8] Malmberg, J. and Wharton, C. Collisionless damping of electrostatic plasma waves. Phys. Rev. Lett. 13, 6 (1964), 184–186.
[9] Villani, C. Landau damping. CEMRACS 2010 lectures.
[10] Mouhot, C. ; Villani, C. On Landau damping, Acta Mathematica 207 (September 2011), 29-201.
[11] Eliasson, B. Outflow boundary conditions for the Fourier transformed one-dimensional Vlasov-Poisson system. J. Sci. Comput. 16 (2001), no. 1, 1–28.

In [36] we construct a new set of discrete differential forms based on B-splines of arbitrary degree as well as an associated Hodge operator. The theory is first developed in 1D and then extended to multi-dimension using tensor products. We link our discrete differential forms with the theory of chains and cochains. The spline discrete differential forms are then applied to the numerical solution of Maxwell's equations.

The notion of B-spline based discrete differential forms is recalled and along with a Finite Element Hodge operator, it is used in [35] to design new numerical methods for solving the Vlasov-Poisson equations.

6.7. Simulations of highly oscillatory Vlasov-Poisson system

Participants: E. Frénod, S. Hirstoaga, M. Lutz, E. Sonnendrücker.

In paper [45] a Lie Transform method is applied for a charged beam under the action of a radial external electric field. The aim of the Lie transform method that is used here is to construct a change of variable which transforms the 2D kinetic problem into a 1D problem. This reduces the dimensionality of the problem and make it easier to solve numerically.

In paper [41], in the framework of a Particle-In-Cell scheme for some 1D Vlasov-Poisson system depending on a small parameter, we propose a time-stepping method which is numerically uniformly accurate when the parameter goes to zero. Based on an exponential time differencing approach, the scheme is able to use large time steps with respect to the typical size of the fast oscillations of the solution.

6.8. Waterbag models: analysis and simulations

Participant: N. Besse.

Ion temperature gradient instabilities play a major role in the understanding of anomalous transport in core fusion plasmas. In the considered cylindrical geometry, ion dynamics is described in [20] using a drift-kinetic multi-water-bag model for the parallel velocity dependency of the ion distribution function. In a first stage, global linear stability analysis is performed. From the obtained normal modes, parametric dependencies of the main spectral characteristics of the instability are then examined. Comparison of the multi-water-bag results with a reference continuous Maxwellian case allows us to evaluate the effects of discrete parallel velocity sampling induced by the Multi-Water-Bag model. Differences between the global model and local models considered in previous works are discussed. Using results from linear, quasilinear, and nonlinear numerical simulations, an analysis of the first stage saturation dynamics of the instability is proposed, where the divergence between the three models is examined.

In paper [21] we present two new codes devoted to the study of ion temperature gradient (ITG) driven plasma turbulence in cylindrical geometry using a drift-kinetic multi-water- bag model for ion dynamics. Both codes were developed to complement the Runge–Kutta semi-lagrangian multi-water-bag code GMWB3D-SLC described in [1]. The CYLGYR code is an eigenvalue solver performing linear stability analysis from given mean radial profiles. It features three resolution schemes and three parallel velocity response models (fluid, multi-water-bag, continuous Maxwellian). The QUALIMUWABA quasilinear code is an initial value code allowing the study of zonal flow influence on drift-waves dynamics. Cross-validation test performed between the three codes show good agreement on both temporal and spatial characteristics of unstable modes in the linear growth phase.

6.9. Full wave modeling of lower hybrid current drive in tokamaks

Participants: Takashi Hattori, Simon Labrunie, Jean R. Roche.

This work is performed in collaboration with Yves Peysson (DRFC, CEA Cadarrache). Since September 2012 this work is included in the ANR CHROME.

The aim of this project is to develop a finite element numerical method for the full-wave simulation of electromagnetic wave propagation in plasma. Full-wave calculations of the LH wave propagation is a challenging issue because of the short wave length with respect to the machine size. In the continuation of the works led in cylindrical geometry , a full toroidal description for an arbitrary poloidal cross-section of the plasma has been developed.

Since its wavelength λ at the LH frequency is very small as compared to the machine size R, a conventional full wave description represents a considerable numerical effort.Therefore, the problem is addressed by an appropriate mathematical finite element technique, which incorporates naturally parallel processing capabilities. It is based on a mixed augmented variational (weak) formulation taking account of the divergence constraint and essential boundary conditions, which provides an original and efficient scheme to describe in a global manner both propagation and absorption of electromagnetic waves in plasmas.

With such a description, usual limitations of the conventional ray tracing related to the approximation $\lambda \ll \phi_B \ll R$, where ϕ_B is the size of the beam transverse to the rf power flow direction, may be overcome. Since conditions are corresponding to $\lambda \ll \phi_B \sim R$, the code under development may be considered as a WKB full wave, dielectric properties being local.

This formulation provides a natural implementation for parallel processing, a particularly important aspect when simulations for plasmas of large size must be considered.

The domain considered is as near as possible of the cavity fill by a tokomak plasma. Toroidal coordinates are introduced. In our approach we consider Fourier decomposition in the angular coordinate to obtain stationary Maxwell equations in a cross-section of the tokamak cavity.

A finite element method is proposed for the simulation of time-harmonic electromagnetic waves in a plasma, which is an anisotropic medium. The approach chosen here is sometimes referred to as *full-wave modeling* in the literature: the original Maxwell's equations are used to obtain a second order equation for the time-harmonic electric field. These are written in a weak form using a augmented variational formulation (AVF), which takes into account the divergence. The variational formulation is then discretized using modified Taylor-Hood (nodal) elements.

The analyze of the model considered, existence and unicity of solution, equivalence of the formulation for the domain decomposition formulation was completed in the frame of Takashi Hattori Phd thesis.

During 2013 we continue to develop the domain decomposition method introduced in 2012 and a new preconditioned system was considered in the code "FullWaveFEM", [31].

6.10. Eulerian simulations of parallel transport in the SOL

Participants: S. Hirstoaga, G. Manfredi.

During the year 2013, we have progressed in the implementation of an asymptotic preserving (AP) Eulerian Vlasov code (`VESPA: Vlasov Eulerian Simulator of PArallel transport`) for the study of parallel transport in the scrape-off layer of tokamaks. An AP Vlasov-Poisson code had already been partially developed for the quasi-neutral regime. In this case the small parameter is the Debye length λ (normalized to the parallel connection length). The Poisson equation becomes singular when $\lambda \to 0$: the AP solution consists in reformulating Poisson's equation in a way that is no longer singular in this limit. In theory, any value of λ can be used, including $\lambda = 0$, without numerical instability and without any constraint on the grid spacing and time-step. In practice, we have observed a CFL stability condition (although not very restrictive) and a limit on the smallness of λ. During the past year, we have performed systematic tests on the code, which is now capable of attaining very small values of λ, down to 10^{-4} or even lower. Meaningful results can be obtained with just 1-2 hours of computation on a standard desktop computer (see for example [29]).

The next upgrade of the VESPA code concerns the modelling of collisions, which have been implemented through a relaxation (BGK) term that also retains the possibility to include ionization and recombination in the model. The BGK term has been tested and validated against analytical results. In particular, the AP scheme had to be modified in order to correctly treat the BGK term. These upgrades are now fully integrated into the VESPA code.

Using the VESPA code, we have studied the dynamical response of a stationary sheath-presheath system to an external perturbation, which takes the form of a small density disturbance in the central region of the plasma, far from the sheaths. The numerical results suggest that, for most regimes of physical interest, the perturbation is damped away before it reaches the wall and does not have a significant impact on the structure of the sheath. This scenario has been studied for different temperatures and density profiles of the disturbance.

We have started to look at the impact of secondary electrons (SE) on the structure and the formation of the sheath. SEs were neglected in previous versions of the code but can play a significant role on the wall potential. In the VESPA code, they are now modelled as a Maxwellian electron source located near the wall. First results indicate that a large yield rate of SEs reduces the potential drop between the plasma bulk and the wall.

6.11. Other application domains

6.11.1. Applications of Two-Scale numerical methods

Participant: E. Frénod.

In paper [37] we consider a model for short term dynamics of dunes in tidal area. We construct a Two-Scale Numerical Method based on the fact that the solution of the equation which has oscillations Two-Scale converges to the solution of a well-posed problem. This numerical method uses on Fourier series.

In [18] we present Chapman–Enskog and Hilbert expansions applied to the $O(v/c)$ Boltzmann equation for the radiative transfer of neutrinos in core-collapse supernovae. Based on the Legendre expansion of the scattering kernel for the collision integral truncated after the second term, we derive the diffusion limit for the Boltzmann equation by truncation of Chapman–Enskog or Hilbert expansions with reaction and collision scaling. We also give asymptotically sharp results obtained by the use of an additional time scaling. The diffusion limit determines the diffusion source in the *Isotropic Diffusion Source Approximation (IDSA)* of Boltzmann's equation for which the free streaming limit and the reaction limit serve as limiters. Here, we derive the reaction limit as well as the free streaming limit by truncation of Chapman–Enskog or Hilbert expansions using reaction and collision scaling as well as time scaling, respectively. Finally, we motivate why limiters are a good choice for the definition of the source term in the IDSA.

6.11.2. Inverse problem governed by Maxwell equations

Participant: Jean R. Roche.

This work is performed in collaboration with José Herskovits Norman of UFRJ, Rio de Janeiro, Antonio André Novotny from the LNCC, Petropolis, both from Brazil and Alfredo Canelas from the University of the Republic, Montevideo, Uruguay.

The industrial technique of electromagnetic casting allows for contactless heating, shaping and controlling of chemical aggressive, hot melts. The main advantage over the conventional crucible shape forming is that the liquid metal does not come into contact with the crucible wall, so there is no danger of contamination. This is very important in the preparation of very pure specimens in metallurgical experiments, as even small traces of impurities, such as carbon and sulphur, can affect the physical properties of the sample. Industrial applications are, for example, electromagnetic shaping of aluminum ingots using soft-contact confinement of the liquid metal, electromagnetic shaping of components of aeronautical engines made of superalloy materials (Ni,Ti, etc.), control of the structure solidification.

The electromagnetic casting is based on the repulsive forces that an electromagnetic field produces on the surface of a mass of liquid metal. In the presence of an induced electromagnetic field, the liquid metal changes its shape until an equilibrium relation between the electromagnetic pressure and the surface tension is satisfied. The direct problem in electromagnetic casting consists in determining the equilibrium shape of the liquid metal. In general, this problem can be solved either directly studying the equilibrium equation defined on the surface of the liquid metal, or minimizing an appropriate energy functional. The main advantage of this last method is that the resulting shapes are mechanically stable.

The inverse problem consists in determining the electric currents and the induced exterior field for which the liquid metal takes on a given desired shape. This is a very important problem that one needs to solve in order to define a process of electromagnetic liquid metal forming.

In a previous work we studied the inverse electromagnetic casting problem considering the case where the inductors are made of single solid-core wires with a negligible area of the cross-section. In a second paper we considered the more realistic case where each inductor is a set of bundled insulated strands. In both cases the number of inductors was fixed in advance, see [61]. In order to look for configurations of inductors considering different topologies we introduce a new formulation for the inverse problem using a shape functional based on the Kohn-Vogelius criterion. A topology optimization procedure is defined by means of topological derivatives, a new method that simplifies computation issues was considered, see [60] and [49].

During 2013 we rewrite the inverse electromagnetic casting model in order to have a quadratic programming problem, this simplified the numerical solution and simulation [19].

CONCHA Project-Team

6. New Results

6.1. New result 1

MICMAC Project-Team

5. New Results

5.1. Electronic structure calculations

Participants: Eric Cancès, Ismaila Dabo, Virginie Ehrlacher, David Gontier, Salma Lahbabi, Claude Le Bris, Gabriel Stoltz.

In electronic structure calculation as in most of our scientific endeavours, we pursue a twofold goal: placing the models on a sound mathematical grounding, and improving the numerical approaches.

E. Cancès and S. Lahbabi have addressed issues related to the modeling and simulation of defects in periodic crystals. Computing the energies of local defects in crystals is a major issue in quantum chemistry, materials science and nano-electronics. In collaboration with M. Lewin (CNRS, Cergy), E. Cancès and A. Deleurence have proposed in 2008 a new model for describing the electronic structure of a crystal in the presence of a local defect. This model is based on formal analogies between the Fermi sea of a perturbed crystal and the Dirac sea in Quantum Electrodynamics (QED) in the presence of an external electrostatic field. The justification of this model is obtained using a thermodynamic limit of Kohn-Sham type models. In collaboration with M. Lewin, E. Cancès and S. Lahbabi have introduced a functional setting for mean-field electronic structure models of Hartree-Fock or Kohn-Sham types for disordered quantum systems, and used these tools to study the reduced Hartree-Fock model for a disordered crystal where the nuclei are classical particles whose positions and charges are random.

D. Gontier has obtained a complete, explicit, characterization of the set of spin-polarized densities for finite molecular systems. This problem was left open in the pionnering work of von Barth and Hedin setting up the Kohn-Sham density functional theory for magnetic compounds.

On the numerical side, E. Cancès, L. He (ENPC), Y. Maday (University Paris 6) and R. Chakir (IFSTTAR) have designed and analyzed a two-grid methods for nonlinear elliptic eigenvalue problems, which can be applied, in particular, to the Kohn-Sham model. Some numerical tests demonstrating the interest of the approach have been performed with the Abinit software.

Implicit solvation models aims at computing the properties of a molecule in solution (most chemical reactions take place in the liquid phase) by replacing all the solvent molecules but the few ones strongly interacting with the solute, by an effective continuous media accounting for long-range electrostatics. E. Cancès, Y. Maday (Paris 6), and B. Stamm (Paris 6) have recently introduced a very efficient domain decomposition method for the simulation of large molecules in the framework of the so-called COSMO implicit solvation models. A collaboration with F. Lipparini (Paris 6), B. Mennucci (Department of Chemistry, University of Pisa) and J.-P. Picquemal (Paris 6) is in progress to implement this algorithm in widely used computational softwares (Gaussian and Tinker), and to extend this method to other implicit solvation models.

Claude Le Bris, in collaboration with Pierre Rouchon (Ecole des Mines de Paris), has pursued the study of a new efficient numerical approach, based on a model reduction technique, to simulate high dimensional Lindblad type equations at play in the modelling of open quantum systems. The specific case under consideration is that of oscillation revivals of a set of atoms interacting resonantly with a slightly damped coherent quantized field of photons. The approach may be employed for other similar equations. Current work is directed towards other numerical challenges for this type of problems.

5.2. Computational Statistical Physics

Participants: Claude Le Bris, Frédéric Legoll, Tony Lelièvre, Francis Nier, Mathias Rousset, Gabriel Stoltz.

5.2.1. Free Energy calculations

For large molecular systems, the information of the whole configuration space may be summarized in a few coordinates of interest, called reaction coordinates. An important problem in chemistry or biology is to compute the effective energy felt by those reaction coordinates, called free energy.

In [39], T. Lelièvre and G. Stoltz, in collaboration with physicists from CEA Saclay (especially, M. Athenes) studied a new adaptive technique of ABF type to compute on-the-fly the free energy of a system, without evaluating the second derivatives of the reaction coordinate. The method uses a Bayesian reinterpretation of an extended system where the reaction coordinate is considered as an additional variable.

In [44], G. Fort (Telecom Paris), B. Jourdain (CERMICS), E. Kuhn (INRA), T. Lelièvre and G. Stoltz have studied the efficiency of the Wang-Landau algorithm, building on a previous study where they proved the convergence of this method. The aim was to obtain precise estimates of the exit times out of metastable states. This was done in two ways: a theoretical study in the simplest possible metastable situation, a system with three states; and a numerical study in a more realistic situation (a two-dimensional double well potential).

5.2.2. Sampling trajectories

There exist a lot of methods to sample efficiently Boltzmann-Gibbs distributions. The situation is much more intricated as far as the sampling of trajectories (and especially metastable trajectories) is concerned.

Recently, the quasi stationary distribution has been identified by the team as a good mathematical tool to analyze metastable trajectories, and to make a link between a continuous state space dynamics (Langevin dynamics) and a discrete state space dynamics (kinetic Monte Carlo models), see for examplelelievre-13. This perspective can also be used to analyze accelerated dynamics techniques which have been proposed by A. Voter in the late nineties, to simulate very efficiently the state-to-state dynamics associated with metastable trajectories. For example, in [33], T. Lelièvre with D. Aristoff (University of Minnesota) propose a mathematical analysis of the Temperature Accelerated Dynamics. In [49], T. Lelièvre and F. Nier have studied the quasi-stationary distribution for an overdamped Langevin process in a bounded domain. In the small temperature limit and by making the connection with boundary Witten Laplacians, they are able to accurately compute the spatial exit law along the boundary and non perturbative accurate formulas when the potential is changed inside the domain. This gives some insight into the foundations of the hyperdynamics method.

Finally, following a numerical observation in a previous work on the sampling of reactive trajectories by a multilevel splitting algorithm, F. Cérou (Inria Rennes), A. Guyader (Inria Rennes), T. Lelièvre and F. Malrieu (Université de Rennes) study theoretically in [19] the distribution of the lengths of these trajectories, using large deviation techniques.

5.2.3. Nonequilibrium systems

Let us also mention that the article [22] on a derivation of a Langevin-type dynamics for a heavy particle in a non-zero background flow, co-authored by M. Dobson, F. Legoll, T. Lelièvre, and G. Stoltz, has been published.

5.2.4. Sampling techniques

In [29], T. Lelièvre studies with F. Nier and G. Pavliotis (Imperial College, London) the interest of using non-reversible dynamics (overdamped Langevin dynamics with a non-gradient drift term) to efficiently sample a given Boltzmann-Gibbs distribution.

5.2.5. Numerical analysis of simulation methods

Together with B. Leimkuhler and Ch. Matthews (Edinburgh University), G. Stoltz studied in [48] the discretization errors in the computation of average properties with Langevin dynamics integrated with splitting strategies. The average properties are either static (average of a given observable) or dynamic (transport coefficients). The main tool used in this analysis is the expansion of the transition operator in powers of the time step, with exact integral remainders; as well as fine estimates on the resolvent of the Langevin operators,

especially in the so-called overdamped limit where the friction goes to infinity. Transport coefficients are studied either through errors in Green-Kubo formulae or errors in the linear response of nonequilibrium systems.

5.2.6. Coarse-graining of molecular systems

G. Stoltz, in collaboration with J.-B. Maillet and G. Faure, developed in [43] a potential energy function depending on the local density of the molecular fluid. The local density is evaluated with a three dimensional Voronoi tesselation, which proves more rigorous than the standard local averages typically found in the literature. The new potential allows to describe the compressibility of mesoparticles representing several molecules in a coarse-grained description of the atomic system. The quality of the potential has been assessed by reproducing equations of state and Hugoniot curves of model energetic materials.

5.2.7. Thermodynamic limit

The quasicontinuum method is an approach to couple an atomistic model with a coarse-grained approximation in order to compute the states of a crystalline lattice at a reduced computational cost compared to a full atomistic simulation. In that framework, the team has addressed questions related to the *finite temperature* modeling of atomistic systems and derivation of coarse-grained descriptions, such as canonical averages of observables depending only on a few variables. The work from F. Legoll and X. Blanc (Université Pierre et Marie Curie) is now published [12].

When the temperature is small, a perturbation approach can be used to compute the canonical averages of these observables depending only on a few variables, at first order with respect to temperature. The work from F. Legoll in collaboration with E. Tadmor, W. K. Kim, L. Dupuy and R. Miller on the analysis of such an approach is now also published [32].

5.2.8. Hamiltonian dynamics

Constant energy averages are often computed as long time limits of time averages along a typical trajectory of the Hamiltonian dynamics. One difficulty of such a computation is the presence of several time scales in the dynamics: the frequencies of some motions are very high (e.g. for the atomistic bond vibrations), while those of other motions are much smaller. This problem has been addressed in a two-fold manner.

Fast phenomena are often only relevant through their mean effect on the slow phenomena, and their precise description is not needed. The work from M. Dobson, C. Le Bris, and F. Legoll developing integrators for Hamiltonian systems with high frequencies (derived using homogenization techniques applied to the Hamilton-Jacobi PDE associated to the Hamiltonian ODE) is now published [22].

Another track to simulate the system for longer times is to resort to parallel computations. An algorithm in that vein is the parareal in time algorithm. The work from C. Le Bris and F. Legoll, in collaboration with X. Dai and Y. Maday, studying several variants of the original plain parareal in time algorithm, is now also published [21].

5.2.9. Effective dynamics

For a given molecular system, and a given reaction coordinate $\xi : \mathbb{R}^n \mapsto \mathbb{R}$, the free energy completely describes the statistics of $\xi(X)$ when $X \in \mathbb{R}^n$ is distributed according to the Gibbs measure. On the other hand, obtaining a correct description of the dynamics along ξ is complicated. In this context, S. Lahbabi and F. Legoll have studied in [8] the case when the fine-scale, reference dynamics is a kinetic Monte Carlo model with small and fast time scales, and proved a path-wise convergence to a coarse kinetic Monte Carlo model only retaining slow degrees of freedom.

Another question is how to use a coarse-grained description (involving only the slow degrees of freedom) as a predictor for the dynamics of the actual reference system, involving all degrees of freedom. Together with G. Samaey (KU Leuven), F. Legoll and T. Lelièvre have addressed this question in the parareal framework, and shown in [28] that the precise coupling between both models should be done carefully in order for the algorithm to be efficient. In that case, the algorithm converges to the reference full dynamics.

5.3. Complex fluids

Participants: David Benoit, Sébastien Boyaval, Claude Le Bris, Tony Lelièvre.

In his PhD under the supervision of Claude Le Bris and Tony Lelièvre, David Benoit studies models of aging fluids developed at the ESPCI (Ecole supérieure de physique et de chimie industrielles) and designed to take into account phenomena such as shear thinning, aging and shear banding in falling sphere experiments. The work consists in studying on the one hand the mathematical well-posedness of some macroscopic models, see [10], and, on the other hand, in trying to understand the link between such macroscopic models and microscopic models which have been proposed to describe such fluids, see [34].

Let us also mention that the paper [28] on a parareal algorithm to efficiently simulate micro-macro models which has been published this year.

Related to the mathematical modelling of free-surface complex flows under gravity, a new reduced model for thin layers of a viscoelastic upper-convected Maxwell fluid was derived by S. Boyaval in collaboration with François Bouchut. Possibly discontinuous solutions were numerically simulated with a new finite-volume scheme of relaxation type that satisfies a discrete counterpart of the natural dissipation [13].

This work has been pursued for other fluid models and other flow regimes, with a view to better understanding the reduction mechanism leading from a physically detailed model to a useful one for numerical simulations at large (geophysical) scales [35].

On the other hand, note that it is often possible to consider only models for *incompressible* fluids (at low Mach numbers). Now, it is both important and delicate to understand how to numerically discretize the incompressibility constraint, a long-standing issue in numerical fluid mechanics. In collaboration with M. Picasso (EPFL), S. Boyaval has thus investigated the possibility to numerically quantify *a posteriori* the quality of a well-known, "simple" numerical method discretizing the incompressibility constraint, in a simple case [36]. This is part of another effort toward useful numerical simulations of complex flows, inline with current questions focused on discretization methods..

5.4. Application of greedy algorithms

Participants: Sébastien Boyaval, Eric Cancès, Virginie Ehrlacher, Tony Lelièvre.

Model reduction techniques are very important tools for applications. They consist in deriving from a high-dimensional problem, a low-dimensional model, which gives very quickly reliable results. We are in particular interested in two techniques: Proper Generalized Decomposition (greedy algorithms) and Reduced Basis techniques.

Concerning the Proper Generalized Decomposition, current research concerns the approximation of high-dimensional spectral problems, see [38]. Prototypical applications include electronic structure calculations or the computation of buckling modes in mechanics. We also explored in the PhD of J. Infante Acevedo the application of these techniques to option pricing problems, see [45].

Finally, in [40], Fabien Casenave (CERMICS), Alexandre Ern (CERMICS), Guillaume Sylvand (EADS IW) and Tony Lelièvre propose a new non intrusive implementation of the reduced basis technique using the Empirical Interpolation Method. The interest if the method is illustrated on aeroacoustic problems.

5.5. Homogenization and related topics

Participants: Virginie Ehrlacher, Claude Le Bris, Frédéric Legoll, François Madiot, William Minvielle.

The homogenization of (deterministic) non periodic systems is a well known topic. Although well explored theoretically by many authors, it has been less investigated from the standpoint of numerical approaches (except in the random setting). In collaboration with X. Blanc and P.-L. Lions, C. Le Bris has introduced a possible theory, giving rise to a numerical approach, for the simulation of multiscale nonperiodic systems. The theoretical considerations are based on earlier works by the same authors (derivation of an algebra of functions appropriate to formalize a theory of homogenization). The numerical endeavour is completely new. Promising results have been obtained on a simple case of a periodic system perturbed by a localized defect. Ongoing works consider other configurations, such as for instance an interface between two different crystalline phases.

The project-team also has pursued its efforts in the field of stochastic homogenization of elliptic equations, aiming at designing numerical approaches that both are pratically relevant and keep the computational workload limited.

Using the standard homogenization theory, one knows that the homogenized tensor, which is a deterministic matrix, depends on the solution of a stochastic equation, the so-called corrector problem, which is posed on the *whole* space $\mathbb{R}^d$. This equation is therefore delicate and expensive to solve. In practice, the space $\mathbb{R}^d$ is truncated to some bounded domain, on which the corrector problem is numerically solved. In turn, this yields a converging approximation of the homogenized tensor, which happens to be a *random* matrix. For a given truncation of $\mathbb{R}^d$, the team has previously shown that the variance of this matrix can be reduced using the technique of antithetic variables. In [47], F. Legoll and W. Minvielle have extended this technique to nonlinear, convex homogenization problems.

In addition, F. Legoll and W. Minvielle have investigated the possibility to use other variance reduction approaches, such as control variate techniques. A promising idea is to use the weakly stochastic model previously introduced by A. Anantharaman and C. Le Bris (in which a periodic model is perturbed by a *rare* stochastic perturbation) to build a control variate model. The preliminary results that have already been obtained are very encouraging.

Yet another approach to reduce the variance is the so-called Multi Level Monte Carlo (MLMC) approach, which is based on using a surrogate model for the quantity of interest. The MLMC approach consists in using many realizations of the surrogate model (which is cheap to evaluate) and few realizations of the reference model (which is more expensive to evaluate). In collaboration with Y. Efendiev and C. Kronsbein, F. Legoll has explored in [41] how this approach can be used in random homogenization.

We have discussed above approaches to efficiently compute the homogenized coefficient, assuming we have a complete knowledge of the microstructure of the material. We have recently started to consider a related inverse problem, and more precisely a parameter fitting problem. Knowing the homogenized quantities, is it possible to recover some features of the microstructure properties? Obviously, since homogenization is an averaging procedure, not everything can be recovered from macroscopic quantities. A realistic situation is the case when we assume a functional form of the distribution of the microscopic properties, but with some unknown parameters that we would like to determine. In collaboration with A. Obliger and M. Simon, F. Legoll and W. Minvielle have started to address that problem, determining the unknown parameters of the microscopic distribution on the basis of macroscopic (e.g. homogenized) quantities. The preliminary results that have been obtained are very encouraging.

From a numerical perspective, the Multiscale Finite Element Method (MsFEM) is a classical strategy to address the situation when the homogenized problem is not known (e.g. in difficult nonlinear cases), or when the scale of the heterogeneities, although small, is not considered to be zero (and hence the homogenized problem cannot be considered as an accurate enough approximation).

The MsFEM has been introduced more than 10 years ago. However, even in simple deterministic cases, there is actually still room for improvement in many different directions. In collaboration with A. Lozinski (University of Besançon), F. Legoll and C. Le Bris have introduced and studied a variant of MsFEM that considers Crouzeix-Raviart type elements on each mesh element. The continuity across edges (or facets) of the (multiscale) finite element basis set functions is enforced only weakly, using fluxes rather than point values. The approach has been analyzed (combining classical arguments from homogenization theory and finite element theory) and tested on simple, but highly convincing cases [27]. In particular, an elliptic problem set on a domain with a huge number of perforations has been considered in [37]. The variant developed outperforms all existing variants of MsFEM.

A follow up on this work, in collaboration with U. Hetmaniuk (University of Washington in Seattle) and A. Lozinski (University of Besançon), consists in the study of multiscale advection-diffusion problems. Such problems are possibly advection dominated and a stabilization procedure is therefore required. How stabilization interferes with the multiscale character of the equation is an unsolved mathematical question

worth considering for numerical purposes. This is the aim of the PhD thesis of François Madiot, which began in October 2013.

Still another question related to homogenization theory that is investigated in the group is the following. Consider an elliptic equation, say in divergence form, with a highly oscillatory matrix coefficient. Is it possible to approximate the boundary value problem for different right hand sides using a similar problem with a *constant* matrix coefficient? How can this "best" constant matrix approximating the oscillatory problem be constructed in an efficient manner? We have addressed some of these questions in [25], where we have in particular shown that this best constant matrix converges to the homogenized matrix, in the limit of infinitely rapidly oscillatory coefficients. Our approach can therefore be considered as an alternative way to compute the homogenized matrix. This is particularly interesting in random cases, where the standard approach is very expensive. Current work is directed towards extending the approach, in order to compute other quantities of interest than the homogenized coefficient.

To conclude this section, we mention the project undertaken by V. Ehrlacher during her six months postdoctoral position in the Cluster of Excellence Engineering of Advanced Materials (Erlangen University). This project, in collaboration with C. Le Bris, F. Legoll, G. Leugering and M. Stingl, aims at optimizing the shape of some materials (modelled as structurally graded linear elastic materials) in order to achieve the best mechanical response at the minimal cost. As often the case in shape optimization, the solution tends to be highly oscillatory, thus the need of homogenization techniques. We thus consider an initial microstructured material composed of steel and void and whose microstructure pattern is periodic (think e.g. of a periodic honeycomb structure). We next consider materials which are obtained from this initial material through a macroscopic deformation, and look for the optimal deformation achieving the best mechanical response. Encouraging first results have been obtained.

5.6. Coupling methods and variance reduction

Participant: Mathias Rousset.

Recently, M. Rousset has initiated a research topic on variance reduction techniques (called "asymptotic") for the simulation of stochastic models of particles. The point is to use a macroscopic (or model reduced) equation as a control variate; or in other words, to use the information of a macroscopic description to decrease the statistical error of the simulated microscopic evolution.

A first step in this program has been achieved for a microscopic model describing the individual motion of bacteriae with a Markovian velocity-jump process. The macroscopic equation is an advection-diffusion equation called the chemotaxis equation. In [30], the pobabilistic derivation of the chemotaxis equation from the individual motion of bacteriae have been carried out in a rigorous way. In [31], a numerical method simulating the individual evolution of bacteriae with "asymptotic" variance reduction have been proposed.

Motivated by the asymptotic variance reduction of DSMC methods (particle Monte-Carlo methods simulating low density fluids modeled by kinetic equations), the work in [50], M. Rousset considers space homogenous Boltzmann kinetic equations in dimension d with Maxwell collisions (and without Grad's cut-off). An explicit Markov coupling of the associated conservative (Nanbu) stochastic N-particle system is constructed, using plain parallel coupling of isotropic random walks on the sphere of two-body collisional directions. The resulting coupling is almost surely decreasing, and the L_2-coupling creation is computed explicitly. Some quasi-contractive and uniform in N coupling / coupling creation inequalities are then proved, relying on 2 + α-moments ($\alpha > 0$) of velocity distributions; upon N-uniform propagation of moments of the particle system, it yields a N-scalable α-power law trend to equilibrium. The latter are based on an original sharp inequality, which bounds from above the coupling distance of two centered and normalized random variables $(U, V) \in \mathbb{R}^d$, with the average square parallelogram area spanned by $(U - U_*, V - V_*)$, (U_*, V_*) denoting an independent copy. Two counter-examples proving the necessity of the dependance on > 2-moments and the impossibility of strict contractivity are provided. The paper, (mostly) self-contained, does not require any propagation of chaos property and uses only elementary tools.

SCIPORT Team

6. New Results

6.1. Automatic Differentiation and parallel codes

Participants: Valérie Pascual, Laurent Hascoet, Jean Utke [Argonne National Lab. (Illinois, USA)], Michel Schanen [RWTH Aachen University (Germany)].

Together with colleagues in Argonne National Lab. and RWTH Aachen, we are studying how AD tools can handle MPI-parallel codes, especially in adjoint mode. Results are progressively incorporated into a library (AMPI, for Adjoinable-MPI) that is designed to provide efficient tangent and adjoint differentiation for MPI-parallel codes, independently of the AD tool used (AdolC, dco, OpenAD, TAPENADE ...). Primitives from the AMPI library dynamically orchestrate, at run-time, the MPI calls that are needed to compute the derivatives.

This year we studied issues raised by the collective reduction operations of MPI, and by the one-sided communications (i.e. remote memory access) offered by MPI-II.

The participants met on two occasions, two weeks in march in Sophia-Antipolis, and two weeks in october in Argonne.

This work was presented in particular at the meeting of the Inria-Illinois joint lab in june in Lyon. An article is in preparation.

6.2. Automatic Differentiation and Dynamic Memory

Participants: Valérie Pascual, Laurent Hascoet, Jean Utke [Argonne National Lab. (Illinois, USA)].

Adjoint differentiated code obtained by source transformation (OpenAD, TAPENADE...) consists of a forward sweep that essentially copies the original code, and a backward sweep that computes the derivatives, These two sweeps must have the same control flow shape, only reversed. The allocation and deallocation of some dynamic memory inside the forward sweep requires a similar pattern in the backward sweep. However, allocations do not always return the same memory chunk, and therefore all memory addresses must be updated to preserve their consistency in the backward sweep.

This problem can only be solved dynamically, at run-time. A compile-time analysis would have to be conservative, implying many overapproximations and in the end an unreasonably inefficient adjoint code. Our approach is thus to design a library that encapsulates all calls to memory allocation primitives (`malloc`, `free`...) in order to register the allocated addresses and to be able to restore consistency of pointers during the backward sweep. This strategy is similar to the one we use for MPI calls, *cf* 6.1 , and is actually needed in our AMPI strategy. All we can hope from a static analysis is to detect the simple cases where addresses could be recomputed instead of stored and updated. This may apply to a significant portion of memory manipulalions, and may thus reduce the overhead due to the dynamic updating.

We started developing this library, called ADMM for Adjoinable Dynamic Memory Management. TAPENADE will eventually produce adjoint code that calls these primitives instead of the standard memory management primitives.

6.3. Automatic Differentiation and iterative processes

Participants: Laurent Hascoet, Ala Taftaf.

Adjoint codes naturally propagate partial gradients backwards from the result of the simulation. However, this uses the data flow of the simulation in reverse order, at a cost that increases with the length of the simulation. AD research looks for strategies to reduce this cost, taking advantage of the structures of the given program. One such structure is iterative fixed point loops, commonplace in numerical computation. They occur at the topmost level of steady-state simulations, as well as in unsteady simulations. They may also occur deeper in the simulation, for instance in linear solvers.

It clear that the first iterations of a fixed-point search operate on a meaningless state vector, and that reversing the corresponding data-flow is wasted effort. An adapted adjoint strategy for the iterative process should consider only the last or the few last iterations. Furthermore, there is a discrete component to an iterative algorithm, namely the number of iterations, and this makes differentiability questionnable. For these reasons we are looking for a specific strategy for the adjoint, that reverses only the necessary data-flow, and that restores confidence in the validity of the derivative.

We seek inspiration in the strategies proposed by two authors [19], [27] to design one strategy that is amenable to implementation in a source-transformation AD tool such as TAPENADE. This will be triggered by user-given differentiation directives. We are also selecting example codes (a steady-state flow solver and a Newton solver) to benchmark and experiment.

Ala Taftaf presented her preliminary results at Queen Mary University in september, and at the 13th EuroAD workshop in Oxford, december 9-10. She attended a training on the CFD code OpenFOAM at Queen Mary, september 3-6.

6.4. Differentiation of third-party codes

Participants: Valérie Pascual, Laurent Hascoet, Alain Dervieux.

This year, we have differentiated two applications brought to us by academic colleagues. This is an important activity as it points us to problems that should be solved or interfaces that should be improved in TAPENADE.

- Striation simulates ionospheric plasma. It was developed in the University of Lille, then Toulouse. The Fortran90 source is relatively compact (10,000 lines). We obtained and validated the tangent and adjoint derivatives that were needed to solve an inverse problem i.e., identify the initial condition that causes an observed instability in plasma density. This work uncovered important AD issues when dynamic memory is used intensively, *cf* 6.2 .
- Mascaret is a hydrodynamic simulation code developed and used by EDF to study river flows. Mascaret consists of 120,000 lines of Fortran90. In this first experiment, we differentiated only one of the three kernel solvers. We obtained validated tangent and adjoint derivatives. A further collaboration with EDF and CERFACS is planned next year.

In addition, Automatic Differentiation of the CFD code AIRONUM (*cf* 5.1) will continue in cooperation with the partners of the FP7 project UMRIDA.

6.5. Resolution of linearised systems

Participants: Hubert Alcin [Inria Bordeaux-Sud-Ouest], Olivier Allain [Lemma], Marianna Braza [IMF-Toulouse], Alexandre Carabias, Alain Dervieux, Bruno Koobus [Université Montpellier 2], Carine Moussaed [Université Montpellier 2], Stephen Wornom [Lemma].

The work of Hubert Alcin for the ANR ECINADS on scalable parallel solvers based on coarse grids has been continued by Carine Moussaed and Bruno Koobus. This results in scalable computations up to 2048 processors.

Bruno Koobus and Carine Moussaed presented their results on “Un modèle VMS-LES dynamique pour la simulation d’écoulements autour d’obstacles” at CANUM congress, Super-Besse, France, May 21-25.

6.6. Control of approximation errors

Participants: Alexandre Carabias, Gautier Brethes, Alain Dervieux, Adrien Loseille [Gamma3 team, Inria-Rocquencourt], Frédéric Alauzet [Gamma3 team, Inria-Rocquencourt], Estelle Mbinky [Gamma3 team, Inria-Rocquencourt], Stephen Wornom [Lemma], Olivier Allain [Lemma], Anca Belme [university of Paris 6].

Third-order mesh adaptation was the main topic of the year in error control. Two PhD have been completed this year on third-order mesh adaptation:

- In team Gamma3, Estelle Mbinky has studied a method from Bernard Mourrain for transforming trilinear Taylor terms of the approximation error into a power of a bilinear term. Estelle Mbinky defended her thesis at Paris 6 on december 20.
- In our team, Alexandre Carabias (who spent most of this year with team Gamma3) has developed a 2D third-order scheme for the Euler model. The scheme is based on the ENO finite-volume formulation with quadratic reconstruction. Some effort was devoted to improve the performance of the scheme. The scheme is much less dissipative than an usual quadratic ENO scheme and of smaller cost. Implementation of a 3D version in AIRONUM (*cf* 5.1) is now starting. The 2D scheme has been the basis of an investigation of third order anisotropic mesh adaptation. Alexandre Carabias defended his thesis in Sophia-Antipolis on december 12.

A. Carabias and E. Mbinky presented their work on "A priori-based mesh adaptation for third-order accurate Euler simulation" at HONOM 2013, Bordeaux, France, March 18-22. We further studied mesh adaptation for viscous flows and we are preparing a journal article in collaboration with Gamma3 and University of Paris 6.

This year's new topic is the combination of Multi-Grid and anisotropic mesh adaption, with the starting PhD of Gautier Brèthes. The study involves several problematics, and in particular stopping criteria and construction of correctors. This was supported by the ANR project ECINADS, ended in november, but continues with the ANR project MAIDESC (started in october, coordinated by our team) following on mesh adaption and in particular meshes for interfaces, third-order accuracy, meshes for boundary layers, and curved meshes.

SIMPAF Project-Team

6. New Results

6.1. Quantitative homogenization theory

In collaboration with S. Neukamm and F. Otto, A. Gloria developed in [46] and [45] a quantitative approach of the stochastic homogenization of discrete elliptic equations. There are two main achievements. In [46] we developed a general theory which quantifies optimally in time the decay of the non-constant coefficients semi-group associated with discrete random diffusion coefficients satisfying a spectral gap assumption (namely, the environment seen from the particle). Combined with spectral theory this allowed us to make a sharp numerical analysis of the popular periodization method to approximate homogenized coefficients. In [45], we obtained a quantitative two-scale expansion result, and essentially proved that the difference between the solution of a (discrete) elliptic equation with random coefficients on the torus and the first two terms of the two-scale expansion scales as in the periodic case (except in dimension 2, for which there is a logarithmic correction).

6.2. Corrosion

The Diffusion Poisson Coupled Model [32] is a model of iron based alloy in a nuclear waste repository. It describes the growth of an oxide layer in this framework. The system is made of a Poisson equation on the electrostatic potential and convection-diffusion equations on the densities f charge carriers (electrons, ferric cations and oxygen vacancies), supplemented with coupled Robin boundary conditions. The DPCM model also takes into account the growth of the oxide host lattice and its dissolution, leading to moving boundary equations. In [44], C. Chainais-Hillairet and I. Lacroix-Violet consider a simplified version of this model, where only two charge carriers are taken into account and where there is no evolution of the layer thickness. They prove the existence of a steady-state solution to this model. More recently, C. Chainais-Hillairet and I. Lacroix-Violet have also obtained an existence result for the time-dependent simplified model. This result is submitted for publication [47].

P.-L. Colin, C.Chainais-Hillairet and I. Lacroix-Violet have recently performed the numerical analysis of the numerical scheme presented in [31]. The scheme is a Euler implicit in time scheme with Scharfetter-Gummel approximation of the convection-diffusion fluxes. They prove existence of a solution to the scheme, a priori estimates satisfied by the solution and convergence of the numerical scheme to a weak solution of the corrosion model.

Numerical experiments done for the simulation of the full DPCM model with moving boundaries shows the convergence in time towards a pseudo-steady-state. T. Gallouët has proposed a new scheme in order to compute directly this pseudo-steady-state. This scheme has been implemented in the code CALIPSO (ANDRA). Validation is in progress, as the numerical analysis of the scheme.

6.3. New results on finite volume schemes

In [5], C. Chainais-Hillairet, S. Krell and A. Mouton develop Discrete Duality Finite Volume methods for the finite volume approximation of a system describing miscible displacement in porous media (Peaceman model). They establish relevant a priori estimates satisfied by the numerical solution and prove existence and uniqueness of the solution to the scheme. They show the efficiency of the schemes through numerical experiments. Recently, they also proved the convergence of the DDFV scheme for the Peaceman model. This work will be soon submitted for publication.

In [35], M. Bessemoulin-Chatard, C. Chainais-Hillairet and F. Filbet prove several discrete Gagliardo-Nirenberg-Sobolev and Poincaré-Sobolev inequalities for some approximations with arbitrary boundary values on finite volume meshes. The keypoint of their approach is to use the continuous embedding of the space $BV(\Omega)$ into $L^{N/(N-1)}(\Omega)$ for a Lipschitz domain $\Omega \subset \mathbb{R}^N$, with $N \geq 2$. Finally, they give several applications to discrete duality finite volume (DDFV) schemes which are used for the approximation of nonlinear and on isotropic elliptic and parabolic problems.

In [22], M. Bessemoulin-Chatard, C. Chainais-Hillairet and M.-H. Vignal consider the numerical approximation of the classical time-dependent drift-diffusion system near quasi-neutrality by a fully implicit in time and finite volume in space scheme, where the convection-diffusion fluxes are approximated by Scharfetter-Gummel fluxes. They establish that all the a priori estimates needed to prove the convergence of the scheme does not depend on the Debye length λ. This proves that the scheme is asymptotic preserving in the quasi-neutral limit $\lambda \to 0$.

In [24], C. Chainais-Hillairet, A. Jüngel and S. Schuchnigg prove the time decay of fully discrete finite-volume approximations of porous-medium and fast-diffusion equations with Neumann or periodic boundary conditions in the entropy sense. The algebraic or exponential decay rates are computed explicitly. In particular, the numerical scheme dissipates all zeroth-order entropies which are dissipated by the continuous equation. The proofs are based on novel continuous and discrete generalized Beckner inequalities.

6.4. New results in numerical fluid dynamics

In the case of compressible models, as the Euler equations, a careful analysis of sharp and practical stability conditions to ensure the positivity of both density and pressure variables was performed[4]. We are also concerned with the numerical simulation of certain multi-fluids flows, which in particular arises in the modeling of powder/snow avalanches. The hybrid scheme works on unstructured meshes and can be advantageously coupled to mesh refinements strategies in order to follow fronts of high density variation [42]. In particular, we investigate the influence of the characteristics Froude number, Schmidt number and Reynolds number on the front progression. In the context of the PhD thesis of Meriem Ezzoug (University of Monastir, Tunisia), co-advised by C. Calgaro and E. Zahrouni (University of Monastir, Tunisia), we investigate theoretically and numerically the influence of a specific stress tensor, introduced for the first time by Korteweg, in some diffuse interface models which allow to describe some phase transition phenomena, such as surface tension force formulation for multiphase fluid flows. In order to answer these questions, we have developed respectively a Fortran code, a C++ code (NS2DDV-C++, see the softwares section) and a MATLAB code (NS2DDV-M, see the softwares section).

6.5. New results on a posteriori estimates

Some residual-type a posteriori error estimators were developed in the context of magnetostatic and magnetodynamic Maxwell equations, given in their potential and harmonic formulations. Here, the task was to find a relevant decomposition of the error in order to obtain the reliability of the estimator, with the use of ad-hoc interpolations. This work was realized in collaboration with the L2EP Laboratory (Laboratoire d'Electrotechnique et d'Electronique de Puissance de Lille, Lille 1 University), and gave rise to several contributions [7], [18], [19], [20], [21], obtained in the context of the Ph-D thesis and of the Post-doc position of Zuqi Tang. Then, other results about a posteriori error estimators were obtained in other contexts [6], [8]. Recently, we started working on space/time error estimators for finite element methods, arising in the context of low-frequency Maxwell equations (PhD of R. Tittarelli, CIFRE EDF R&D, see [25].

6.6. New results in control in fluid mechanics

Recently, we studied more particularly passive control techniques using porous media for incompressible aerodynamics on several bodies, with the use of the penalisation method [3].

BACCHUS Team

6. New Results

6.1. Residual distribution schemes for steady problems

Participants: Rémi Abgrall [Corresponding member], Mario Ricchiuto, Dante de Santis, Algiane Froehly, Cécile Dobrzynski, Pietro Marco Congedo.

We have understood how to approximate the advection diffusion problem in the context of residual distribution schemes. The third order version of the schemes has been validated for both laminar and turbulent flows. It is uniformly accurate with respect to the local Reynolds number. The turbulent version makes used of extension to the Spalart Allmaras model. We have studied the (iterative) convergence issues using Jacobian Free techniques or the LUSGS algorithm. Tests in two and three dimensions have been carried out. This work is submitted to J.Comput.Phys. We are now able to handle two and three dimensional laminar and turbulent flows on hybrid and high order (curved boundaries) meshes. Moreover, we have extended the scheme to the use of complex equations of state, and we perform high-order computations with real-gas effects. This work is submitted to Computers&Fluids.

6.2. Curved meshes

Participants: Rémi Abgrall, Cécile Dobrzynski [Corresponding member], Algiane Frohely.

One of the main open problems in high order schemes is the design of meshes that fit with enough accuracy the boundary of the computational domain. If this curve/surface is not locally straight/planar, the elements must be curved near the boundary, and their curvature need to be propagated to the interior of the domain to have valid elements. When the mesh is very stretched, this can be quite challenging since, in addition, we want that the mesh keep a structure, in particular for boundary layers. Using tools explored in iso-geometrical analysis, we have been able to construct a software computing curved meshes (in 2D and 3D), while keeping as much as possible the structure of the mesh and guaranteeing that the generated mesh is suitable to CFD simulation (all elements have a positive Jacobian). This software is being used for high order computations with the IDIHOM project. The full paper has been accepted in IJNMF and will be published in 2014.

6.3. Hypoelastic models

Participants: Rémi Abgrall [Corresponding member], Pierre-Henri Maire.

In collaboration with CEA (P.H. Maire), we have developed and tested a new finite volume like algorithm able to simulate hypo-elastic and plastics problems on unstructured meshes. This has been published in [19].

6.4. Penalisation methods using unstructured meshes

Participants: Rémi Abgrall, Heloise Beaugendre [Corresponding member], Cécile Dobrzynski, Leo Nouveau, Quentin Viville.

In Computational Fluid Dynamics the interest on embedded boundary methods for Navier-Stokes equations increases because they simplify the meshing issue, the simulation of multi-physics flows and the coupling of fluid-solid interactions in situation of large motions or deformations. Nevertheless an accurate treatment of the wall boundary conditions remains an issue of these methods. In this work we develop an immersed boundary method for unstructured meshes based on a penalization technique and we use mesh adaption to improve the accuracy of the method close to the boundary. The idea is to combine the strength of mesh adaptation, that is to provide an accurate flow description especially when dealing with wall boundary conditions, to the simplicity of embedded grids techniques, that is to simplify the meshing issue and the wall boundary treatment when combined with a penalization term to enforce boundary conditions. The bodies are described using a level-set method and are embedded in an unstructured grid. Once a first numerical solution is computed mesh adaptation based on two criteria the level-set and the quality of the solution is performed. The full paper will be published in the Journal of Computational Physics in january 2014.

6.5. Unsteady problem

Participants: Rémi Abgrall, Mario Ricchiuto [Corresponding member].

A higher order version of the explicit multi-stage RD schemes we have designed has been obtained in one dimension, and its extension to two space dimensions is in the works. A moving mesh ALE formulation of the multistage explicit schemes developed [58] (paper submitted to J.Sci.Comp.) as a basis for adaptive mesh movement, in development in collaboration with Pr. A. Guardone. We have also started work on new formulations based on different time stepping schemes of the multi-step type.

Concerning implicit schemes, the work on higher order space time formulations in collaboration with the Leeds university and with A. Larat of Ecole Centrale Paris. The advantage of this formulation in terms of efficiency has been shown for shallow water problems [24], while the extension to higher than second order is still in development (Inria RR-7843).

6.6. Uncertainty Quantification

Participants: Rémi Abgrall, Pietro Congedo [Corresponding member], Gianluca Geraci, Maria Giovanna Rodio, Kunkun Tang, Julie Tryoen, Mario Ricchiuto, Thierry Magin.

We developed an unified scheme in the coupled physical/stochastic space. Basing on the Harten multiresolution framework in the stochastic space, we proposed a method allowing an adaptive refinement/derefinement in both physical and stochastic space for time dependent problems (aSI scheme). As a consequence, an higher accuracy is obtained with a lower computational cost with respect to classical non-intrusive approaches, where the adaptivity is performed in the stochastic space only. Performances of this algorithm are tested on scalar Burgers equation and Euler system of equations, comparing with the classical Monte Carlo and Polynomial Chaos techniques [6], [7]. We have also coupled the aSI scheme withe the DEM method for building an accurate stochastic scheme for multiphase flows. A paper is submitted to the Journal of Computational Physics on this topic.

Concerning non-intrusive methods, we proposed a formulation in order to compute the decomposition of high-order statistics. The idea is to compute the most influential parameters for high orders permitting to improve the sensitivity analysis. Second objective is to illustrate the correlation between the high-order functional decomposition and the PC-based techniques, thus displaying how to compute each term from a numerical point of view. This method has been proposed in both classical and Anchored ANOVA representation. Two papers are actually under revision on this topic. Moreover, a bayesian-based method has been used within a Polynomial Chaos framework for rebuilding the freestream conditions, starting from wall measurements during the atmospheric reentry of a space vehicle. See [16] for more details. Moreover, an uncertainty propagation method has been applied to the robust analysis of cavitating flows in a Venturi tube, displaying very interesting results concerning the influence of inlet conditions and the multiphase model parameters (see[23] for more details).

Uncertainty propagation studies are actually underway for assessing the influence of boundary conditions and model parameters for the simulation of a tsunami.

6.7. Robust Design Optimization

Participants: Pietro Congedo [Corresponding member], Gianluca Geraci, Gianluca Iaccarino.

The Simplex-Simplex approach, that has been proposed in 2011, has been further developed. In particular, the algorithm has been improved yielding an evolved version of the Simplex2 approach, and the formulation has been extended to treat mixed aleatory/epistemic uncertainty. The resulting SSC/NM (Simplex Stochastic Collocation/Nelder-Mead) method, called Simplex2, is based on i) a coupled stopping criterion and ii) the use of an high-degree polynomial interpolation of the optimization space. Numerical results show that this method is very efficient for mono-objective optimization and minimizes the global number of deterministic evaluations to determine a robust design. This method is applied to some analytical test cases and to a realistic problem of robust optimization of a multi-component airfoil (see [17] for more details).

Morevoer, we proposed a strategy for multi-objective robust design optimization, with a stochastic dimension reduction based on ANOVA analysis. The developed strategy has been applied to the robust optimization of dense-gas turbines (see [15] for more details).

6.8. Multiphase flows

Participants: Rémi Abgrall [Corresponding member], Pietro Congedo, Maria-Giovanna Rodio.

We developed the numerical solver based on a DEM formulation modified for including viscous effects and a more complex equation of state for the vapor region. The method used is the DEM for the resolution of a reduced five equation model with the hypothesis of pressure and velocity equilibrium , without mass and heat transfer. This method results in a well-posed hyperbolic systems, allowing an explicit treatment of non conservative terms, without conservation error (see [8] for more details). The DEM method directly obtains a well-posed discrete equation system from the single-phase conservation laws, producing a numerical scheme which accurately computes fluxes for arbitrary number of phases. We considered two thermodynamic models , i.e. the SG EOS and the Peng-Robinson (PR) EOS. While SG allows preserving the hyperbolicity of the system also in spinodal zone, real-gas effects are taken into account by using the more complex PR equation. The higher robustness of the PR equation when coupled with CFD solvers with respect to more complex and potentially more accurate multi-parameter equations of state has been recently discussed. In this paper, no mass transfer effect is taken into account, thus the PR equation can be used only to describe the vapor behavior, while only the SG model is used for describing the liquid [22].

Another topic covered by Bacchus is about the numerical approximation of non conservative systems. One very interesting example is obtained by the Kapila model, for which shock relations can be found from physical principles. Most, if not all, the know discretisation are at best stable, but do not converge under mesh refinement. We have proposed a way to do so by using some modifications of a Roe-like solver.

6.9. Depth averaged free surface modeling

Participants: Mario Ricchiuto [Corresponding member], Philippe Bonneton, Andrea Filippini, Stevan Bellec.

We have improved the modeling capabilities of our codes by an efficient implementation of residual based dicretizations of a non-hydrostatic enhanced Boussinesq system [21]. in particular, we have demonstrated how residual based stabilization terms do not pollute the accuracy of the underlying centered discretization, and lead very low dispersion error, while allowing to handle in a stable manner the hyperbolic (hydrostatic) limit. In the framework of the internship of P. Bagicaluppi, this has been used to construct a non-oscillatory model including wave breaking effects (paper in preparation).

In parallel, we have started an in depth study of the improvement of the dispersion operators, which control the position and height of the waves. This has allowed to highlight the existence of new form of weakly nonlinear models [62]. A paper is in preparation.

6.10. Self healing composites modeling

Participants: Mario Ricchiuto [Corresponding member], Gérard Vignoles, Gregory Perrot.

This year we have started the coupling between `COCA` and the structural solver of the LCTS lab. The coupling is done for the moment using simple scripting, and providing the structural solver with an equivalent fiber-surface in contact with oxygen at a given time. A simplified potential flow model (classical source potential) for the oxide has also been developed and is being tested.

6.11. Parallel remeshing

Participants: Cécile Dobrzynski, Cédric Lachat, François Pellegrini [Corresponding member].

All the work of the elapsed year on PaMPA concentrated on the design and implementation of parallel remeshing algorithms (see Section 5.6 for more details about the software itself). These algorithms are based on several steps: (i) identification of the areas to remesh; (ii) splitting of these areas into zones of prescribed size and/or estimated workload; (iii) redistribution and centralization of as many zones as possible on the processors; (iv) sequential remeshing of the zones; (v) reintegration of the zones to their original locations; (vi) identification of the remaining areas and loop to step (ii) when work remains.

Several splitting algorithms have been designed and evaluated, so as to provide zones with adequate aspect ratios to the sequential partitioners. Load imbalance is still a concern, since zones must not be too small, while they must be numerous enough so as to maximize concurrency across all of the available processors.

As of December, PaMPA has been able to remesh a coarse mesh of 27 millions of tetraedra up to a fine mesh comprising more than 600 millions of tetraedra, in 34 minutes, on 240 processors of the Avakas cluster at MCIA Bordeaux, using the MMG3D sequential remesher. Remeshing up to a finer mesh of above one billion of elements is the next milestone to reach, to evidence the capabilities of the software.

Cédric Lachat defended his PhD last December. A first abstract has been submitted, and two more journal papers are in preparation.

Figure 4. Cut of a 3D cube made of tetrahedra showing the effect of parallel remeshing by PaMPA.

6.12. Graph remapping

Participants: Sébastien Fourestier, François Pellegrini [Corresponding member].

The work on remapping mostly took place in the context of the PhD of Sébastien Fourestier, who defended last June. This work concerned the coding and evaluation of the parallel graph repartitioning and remapping algorithms that were designed last year. Indeed, the sequential version of these algorithms had been integrated in version 6.0 of Scotch, released in the beginning of December 2012. The implementation of the parallel algorithms, which started last year, took place in the 6.1 branch of Scotch, to be released once the 6.0 branch is made stable.

The evaluatin of our algorithms showed that the diffusion-based optimization algorithm, which behaves well in the context of partitioning, exhibits an unwanted behavior when adapted to the repartitioning and remapping cases. Typically, when the mapping changes too much, external constraints to the flows that represent the different parts may prevent them from meeting, thus reducing the quality of the frontier they should create by flooding one against the others. These algorithm have to be improved.

A journal paper summing-up all the work done during the past years in the context of process mapping, within the Joint Laboratory for Petascale Computing (JLPC) between Inria and UIUC, has been submitted.

6.13. Sparse matrix reordering for ILU solvers

Participants: Astrid Casadei [HIEPACS project-team, Inria Bordeaux - Sud-Ouest], Sébastien Fourestier, François Pellegrini [Corresponding member].

In the context of ANR `PETALh`, our task is to find ways of reordering sparse matrices so as to improve the robustness of incomplete LU factorization techniques. The path we are following is to favor the diagonal dominance of the matrices corresponding to the subdomains of the Schur complement. Our studies aim at injecting some information regarding off-diagonal numerical values into nested dissection like reordering methods, so as to favor the preservation of high off-diagonal values into either the subdomains or the separators of Schur complement techniques.

The experimental framework had been set-up last year. It consisted in a modified version of the `Scotch` sparse matrix ordering library for computing orderings and of the `HIPS` iterative sparse linear system solver for evaluating them. The text cases used were provided by the industrial partners of the `PETALh` project.

In order to improve diagonal dominance, several cut-off methods have been proposed in order to carve the matrix pattern and speed-up computations towards convergence. These cut-off methods were based on either linear or logarithmic scales, with cut-off values selected according to various distributions.

While some of these methods improve convergence on some restricted classes of matrices, as our first experiments showed last year, no method was able to provide overall improvement on a wide range of matrices. This research path is consequently considered as inefficient. A research report has been written.

6.14. Numerical methods for high altitude aerodynamics and rarefied gas flows

Participants: Luc Mieussens [Corresponding member], Florent Pruvost [IMB, engineer], G. Dechristé [IMB, PhD], N. Hérouard [CEA-CESTA, PhD], Stéphane Brull [IMB], L. Forestier-Coste [IMB, Post Doc].

This activity involves many developments for rarefied gas flow simulations for very different applications, and the design of numerical schemes for high altitude aerodynamics based on some kinetic model :

- the simulation code `CORBIS` (rarefied gases in 2 space dimensions on structured meshes) has been re-engineered : modular form, use of the `git` version control system, modification to use unstructured meshes, MPI/OpenMP hybrid parallelization. Very good performance in terms of scalability and efficiency have been obtained, up to 700 cores.
- a new method to generate locally refined grids in the space of velocities has been proposed and shown to provide CPU time gains of the order of 30 (w.r.t the existing approach). This work has been published in (Baranger *et al., J. Comput. Phys* 257(15), 2014) ;
- the second order Discontinuous Galerkin method has been shown to be more accurate and faster than higher order finite volume methods (up to fourth order) for one-dimensional rarefied gases problems. We have analytically proved that this method is Asymptotic Preserving for the Stokes regime ;
- a new kinetic model for multispecies reacting flows for re-entry applications has been proposed. In this model, the mixture oxygen-nytrogen is described by a kinetic equation, while the minor species (O, NO, N) are described by reaction diffusion equations. The implementation of this model in a full 3D code is under way ;

- we have presented one of the first numerical simulation of the Crookes radiometer ever. This has been obtained with a Cartesian grid approach, with a cut-cell techniques allowing a simplified treatment of moving solid boundaries. This work has been published in the proceedings of the 28th Symposium on rarefied Gas Dynamics ;
- We have proposed a new method to discretize kinetic equations based on a discretization of the velocity variable which is local in time and space. This induces an important gain in term of memory storage and CPU time, at least for 1D problems (this work has been presented in a paper submitted for publication). Two-dimensional extensions are under development ;
- We have shown that the recent method "Unified Gas Kinetic Scheme", proposed by K. Xu to simulate multi-scale rarefied gas flows, can be extended to other fields, like radiative transfer. This approach, based on a simple finite volume technique, is very general and can be easily applied to complex geometries with unstructured meshes. This work has been published in (Mieussens, *et al., J. Comput. Phys* 253(15), 2013).

CAGIRE Team

6. New Results

6.1. DNS of a jet in crossflow: generation of a synthetic turbulent signal and coupling with characteristics based boundary conditions

The implementation of the boundary conditions for DNS of the flow configuration that consists of a jet issuing from an inclined cylindrical hole and discharging into a turbulent crossflow is investigated in the framework of our current participation in the Impact-AE EU funded program. First, a method allowing the generation of turbulent inflow that matches targeted statistics (mean velocity and Reynolds stress tensor components measured on the MAVERIC test facility) has been chosen. On the basis of a study of the main classic methods identified in the literature, it has been considered that the Synthetic Eddy Method (SEM) represents the best compromise between effectiveness and cost, from both a computation and a storage point of view. With this approach, eddy structures are created and injected at the inlet plane of the computational domain. These analytically defined structures are chosen in order to reproduce the most relevant ones present in a turbulent channel flow. The SEM implementation has been considered for (1) a basic form of SEM that does not differentiate the vortices in function of their distance to the wall, and (2) a more elaborated version of the method, denoted SEM-WB, where the inlet plane is split into different zones that accommodate different types of coherent structures according to what is observed in a turbulent boundary layer. In order to prescribe realistic turbulence statistics, the targeted mean velocity and Reynolds stress values of the SEM-WB method were obtained by performing dedicated PIV measurements on the MAVERIC test facility (UPPA). The basic form of the method gives quite satisfactory results. The values of some parameters of the SEM-WB method have still to be adjusted in order to achieve a better convergence rate towards the targeted statistics. In november 2013, the deliverable D2.211 (Confidential) documenting in details this methodology and the results obtained with the related module written in C++ has been issued by the team to the IMPACT-AE office. Assuming that the synthetic turbulent signal is generated in a satisfactory way, one is left with the set-up of the procedure necessary to incorporate this signal into a characteristics based method for handling the boundary conditions at the flow inlet(s). We have developed an approach that proved suitable, in a 1-D configuration so far, to accurately superimpose acoustics and turbulence while preserving the non reflective properties at the inlet boundary [5].

6.2. Low Mach number flows simulations issues

Our activity for developing schemes suitable for the simulation of low Mach number flows considers the two main techniques developed initially for dealing with either zero Mach number flows (pressure-velocity coupling) or compressible flows (density based approach). For the methodology adressing the pressure-velocity coupling, we concentrated on the issue of handling in a semi-implicit way the unsteady set of characteristics based equations at both the outlet and the inlet of a subsonic internal flow. The methodology employed to solve the boundary equations has been designed to mimic the pressure-velocity coupling employed in the interior of the computational domain. The numerical experiments carried out with an acoustic CFL number significantly larger than unity show that the expected reflective and non-reflective behavior is preserved at these boundaries [3].

For the density based approach [6], the Euler or Navier-Stokes equations semi-discretised with a Roe-like flux scheme are analysed using an asymptotic development in power of the Mach number. As expected, this development shows that the inaccuracy at low Mach is due to the bad scaling of the pressure gradient in the momentum equation [20]. In addition, the behaviour of any compressible solver based on that scheme proved to be highly dependent on the geometry of the mesh elements [33]. Several cures to this inaccuracy problem exist in the literature for steady flow calculations. But for unsteady low Mach flows simulations, our numerical experiments with high order discontinuous Galerkine discretisation put into evidence the bad

stability properties of these modified schemes. In order to adress that second issue, a semi-discrete wave equation for the order one pressure in the system has been derived by including the acoustic time scale in the asymptotic development. An analysis of the dissipative terms of this wave equation has been started in order to determine the possible way of regaining good stability properties while ensuring a good accuracy at low Mach.

DEFI Project-Team

6. New Results

6.1. Qualitative methods for inverse scattering problems

6.1.1. A generalized formulation of the Linear Sampling Method

Participants: Lorenzo Audibert, Houssem Haddar.

We proposed and analyzed a new formulation of the Linear Sampling Method that uses an exact characterization of the targets shape in terms of the so-called farfield operator (at a fixed frequency). This characterization is based on constructing nearby solutions of the farfield equation using minimizing sequences of a least squares cost functional with an appropriate penalty term. We first provided a general framework for the theoretical foundation of the method in the case of noise-free and noisy measurements operator. We then explicited applications for the case of inhomogeneous inclusions and indicate possible straightforward generalizations. We finally validated the method through some numerical tests and compare the performances with classical LSM and the factorization methods.

6.1.2. Inverse problems for periodic penetrable media

Participant: Dinh Liem Nguyen.

Imaging periodic penetrable scattering objects is of interest for non-destructive testing of photonic devices. The problem is motivated by the decreasing size of periodic structures in photonic devices, together with an increasing demand in fast non-destructive testing. In this project, we considered the problem of imaging a periodic penetrable structure from measurements of scattered electromagnetic waves. As a continuation of earlier work jointly with A. Lechleiter we considered an electromagnetic problem for transverse magnetic waves (previous work treats transverse electric fields), and also the full Maxwell equations. In both cases, we treat the direct problem by a volumetric integral equation approach and construct a Factorization method.

6.1.3. Transmission Eigenvalues and their application to the identification problem

Participant: Houssem Haddar.

The so-called interior transmission problem plays an important role in the study of inverse scattering problems from (anisotropic) inhomogeneities. Solutions to this problem associated with singular sources can be used for instance to establish uniqueness for the imaging of anisotropic inclusions from muti-static data at a fixed frequency. It is also well known that the injectivity of the far field operator used in sampling methods is related to the uniqueness of solutions to this problem. The frequencies for which this uniqueness fails are called transmission eigenvalues. We are currently developing approaches where these frequencies can be used in identifying (qualitative informations on) the medium properties. Our research on this topic is mainly done in the framework of the associate team ISIP http://www.cmap.polytechnique.fr/~defi/ISIP/isip.html with the University of Delaware. A review article on the state of art concerning the transmission eigenvalue problem has been written in collaboration with F. Cakoni. We also edited a spacial issue of the journal Inverse Problems dedicated to the use of these transmission eigenvalues in inverse problems http://iopscience.iop.org/0266-5611/29/10/100201/. Our recent contributions are the following:

- Together with A. Cossonnière we analyzed the Fredholm properties of the interior transmission problem for the cases where the index contrast changes sign outside the boundary by using a surface integral equation approach.
- With F. Cakoni and N. Chaulet we investigated the asymptotic behaviour of the first transmission eigenvalue of a thin coating with respect to the coating thickness.

6.1.4. The factorization method for inverse scattering problems

6.1.4.1. The factorization method for cracks with impedance boundary conditions

Participant: Houssem Haddar.

With Y. Boukari we used the Factorization method to retrieve the shape of cracks with impedance boundary conditions from farfields associated with incident plane waves at a fixed fre- quency. This work is an extension of the study initiated by Kirsch and Ritter [Inverse Problems, 16, pp. 89-105, 2000] where the case of sound soft cracks is considered. We address here the scalar problem and provide theoretical validation of the method when the impedance boundary conditions hold on both sides of the crack. We then deduce an inversion algorithm and present some validating numerical results in the case of simply and multiply connected cracks [5].

6.1.4.2. The factorization method for EIT with uncertain background

Participants: Giovanni Migliorati, Houssem Haddar.

We extended the Factorization Method for Electrical Impedance Tomography to the case of background featuring uncertainty. This work is based on our earlier algorithm for known but inhomogeneous backgrounds. We developed three methodologies to apply the Factorization Method to the more difficult case of piece-wise constant but uncertain background. The first one is based on a recovery of the background through an optimization scheme and is well adapted to relatively low dimensional random variables describing the background. The second one is based on a weighted combination of the indicator functions provided by the Factorization Method for different realiza- tions of the random variables describing the uncertain background. We show through numerical experiments that this procedure is well suited to the case where many realizations of the measurement operators are available. The third strategy is a variant of the previous one when measurements for the inclusion-free background are available. In that case, a single pair of measurements is sufficient to achieve comparable accuracy to the deterministic case [15].

6.1.4.3. The factorization method for GIBC

Participants: Mathieu Chamaillard, Houssem Haddar.

With N. Chaulet, we studied the identification of some obstacle and some Generalized Impedance Boundary Conditions (GIBC) on the boundary of such obstacle from far field measurements generated by the scattering of harmonic incident waves. The GIBCs are approximate models for thin coatings, corrugated surfaces, rough surfaces or imperfectly conducting media.

We justified the use of the Factorization method to solve the inverse obstacle problem in the presence of GIBCs. This method gives a uniqueness proof as well as a fast algorithm to reconstruct the obstacle from the knowledge of the far field produced by incident plane waves for all the directions of incidence at a given frequency. We also provided some numerical reconstructions of obstacles for several impedance operators.

6.2. Iterative Methods for Non-linear Inverse Problems

6.2.1. Inverse medium problem for axisymmetric eddy current models

Participants: Houssem Haddar, Zixian Jiang, Kamel Riahi.

We continued our developments of shape optimization methods for inclusion detection in an axisymmetric eddy current model. This problem is motivated by non-destructive testing methodologies for steam generators. We finalized a joint work with A. Lechleiter on numerical methods for the solution of the direct problem in weighted Sobolev spaces using approriate Dirichlet-to-Neumann mappings to bound the computational domain. We are also finalized jointly with M. El Guedri the work on inverse solver using a regularized steepest descent method for the problem of identifying a magnetite deposits using axial eddy current probe. We then addressed two new issues:

- We developed asymptotic models to identify thin highly conducting deposits. We derived three possible asymptotic models that can be exploited in the inverse problem. The numerical validation is under study.

- We extended the inverse scheeme to 3D configurations with axisymmetry at infinity: this includes exact charactherization of the shape derivative for a mixed formulation of eddy current problems and a parametric inversion scheme based on a pre-defined discrete grid for deposit location.

6.2.2. The conformal mapping method and inverse scattering at low frequencies

Participant: Houssem Haddar.

Together with R. Kress we employed a conformal mapping technique for the inverse problem to reconstruct a perfectly conducting inclusion in a homogeneous background medium from Cauchy data for electrostatic imaging, that is, for solving an inverse boundary value problem for the Laplace equation. In a recent work [13] we proposed an extension of this approach to inverse obstacle scattering for time-harmonic waves, that is, to the solution of an inverse boundary value problem for the Helmholtz equation. The main idea is to use the conformal mapping algorithm in an iterative procedure to obtain Cauchy data for a Laplace problem from the given Cauchy data for the Helmholtz problem. We presented the foundations of the method together with a convergence result and exhibit the feasibility of the method via numerical examples.

6.2.3. A steepest descent method for inverse electromagnetic scattering problems

Participant: Houssem Haddar.

Together with N. Chaulet, we proposed the application of a non linear optimization techniques to solve the inverse scattering problems for the $3D$ Maxwell's equations with generalized impedance boundary conditions. We characterized the shape derivative in the case where the GIBC is defined by a second order surface operator. We then applied a boundary variation method based on a regularized steepest descent to solve the 3-D inverse problem with partial farfield data. The obtained numerical results demonstrated the possibility of identifying the shape of coated objects as well as the parameters of the coating in the $3D$ Maxwell case.

6.3. Shape and topology optimization

6.3.1. Geometric shape optimization

Participant: Grégoire Allaire.

With Ch. Dapogny and P. Frey, we propose a new approach for geometry and topology optimization of structures which benefits from an accurate description of shapes at each stage of the iterative process (by means of a mesh amenable for mechanical analyses) while retaining the whole versatility of the level set method when it comes to accounting for their evolution. The key ingredients of this method are two operators for switching from a meshed representation of a domain to an implicit one, and conversely; this notably brings into play an algorithm for generating the signed distance function to an arbitrary discrete domain, and a mesh generation algorithm for implicitly-defined geometries.

6.3.2. Worst-case design shape optimization

Participant: Grégoire Allaire.

with Ch. Dapogny, we propose a deterministic method for optimizing a structure with respect to its worst possible behavior when a "small" uncertainty exists over some of its features. The main idea is to linearize the considered cost function with respect to the uncertain parameters, then to consider the supremum function of the obtained linear approximation, which can be rewritten as a more classical function of the design, owing to standard adjoint techniques from optimal control theory. The resulting linearized worst-case objective function turns out to be the sum of the initial cost function and of a norm of an adjoint state function, which is dual with respect to the considered norm over perturbations.

6.3.3. Multi-phase structural optimization

Participant: Grégoire Allaire.

With Ch. Dapogny, G. Delgado and G. Michailidis, we consider the optimal distribution of several elastic materials in a fixed working domain. In order to optimize both the geometry and topology of the mixture we rely on the level set method for the description of the interfaces between the different phases. We discuss various approaches, based on Hadamard method of boundary variations, for computing shape derivatives which are the key ingredients for a steepest descent algorithm. The shape gradient obtained for a sharp interface involves jump of discontinuous quantities at the interface which are difficult to numerically evaluate. Therefore we suggest an alternative smoothed interface approach which yields more convenient shape derivatives. We rely on the signed distance function and we enforce a fixed width of the transition layer around the interface (a crucial property in order to avoid increasing "grey" regions of fictitious materials). It turns out that the optimization of a diffuse interface has its own interest in material science, for example to optimize functionally graded materials.

6.3.4. Level-Set Method

Participant: Olivier Pantz.

We have begin to work, with Gabriel Delagado, on a new level-set optimization method, based on a gradient method. The key idea consists in computing directly the derivative of the discretized cost functions. The main advantage is that it is usually more simple to implement than the standard approach (consisting in using a discretized version of the gradient of the cost function). Moreover, the results obtained are as good or even better than the one obtained in previous works. Nevertheless, this method has its drawbacks, since the cost function is only derivable almost everywhere (the zero level-set has to be transverse to the triangulation of the mesh). It follows that convergence toward the minimum by the gradient method is not granted. To overcome this problem, we intend to use a mix-formulation for the state function. Unfortunately, such a formulation, in the case of linear elasticity is quite difficult to obtain. We thus intend to begin with the simplest scalar case, for which a lot more hybrid formulations are available.

6.3.5. Optimization of a sodium fast reactor core

Participants: Grégoire Allaire, Olivier Pantz.

In collaboration with D. Schmidt, G. Allaire and E. Dombre, we apply the geometrical shape optimization method for the design of a SFR (Sodium Fast reactor) core in order to minimize a thermal counter-reaction known as the sodium void effect. In this kind of reactor, by increasing the temperature, the core may become liable to a strong increase of reactivity ρ, a key-parameter governing the chain-reaction at quasi-static states. We first use the 1 group energy diffusion model and give the generalization to the 2 groups energy equation. We then give some numerical results in the case of the 1 group energy equation. Note that the application of our method leads to some designs whose interfaces can be parametrized by very smooth curves which can stand very far from realistic designs. We don't explain here the method that it would be possible to use for recovering an operational design but there exists several penalization methods that could be employed to this end. This work was partially sponsored by EDF. Our results will be published in the proceedings of the CEMRACS'11, during which part of the results have been obtained.

6.4. Asymptotic Analysis

6.4.1. Effective boundary conditions for thin periodic coatings

Participants: Mathieu Chamaillard, Houssem Haddar.

This topic is the object of a collaboration with Patrick Joly and is a continuation of our earlier work on interface conditions done in the framework of the PhD thesis of Berangère Delourme. Th goal here is to derive effective conditions that model scattering from thin periodic coatings where the thickness and the periodicity are of the same length but very small compared to the wavelength. The originality of our work, compared to abundant literature is to consider the case of arbitrary geometry (2-D or 3-D) and to consider higher order approximate models. We formally derived third order effective conditions after exhibiting the full asymptotic expansion of the solution in terms of the periodicity length.

6.4.2. Homogenization of electrokinetic models in porous media

Participant: Grégoire Allaire.

With R. Brizzi, J.-F. Dufrêche, A. Mikelic and A. Piatnitski, we are interested in the homogenization (or upscaling) of a system of partial differential equations describing the non-ideal transport of a N-component electrolyte in a dilute Newtonian solvent through a rigid porous medium. Our work can be divided in two different contributions. First, in the case of an ideal model (for which the homogenized system was already known) we consider the various limits which can be obtained in the effective parameters when the ratio between the characteristic pore length and the Debye length is either small or large. Second, we studied the homogenization process in the non-ideal case, namely when considering the so-called mean spherical approximation (MSA) model which takes into account finite size ions and screening effects.

6.4.3. A new shell modeling modeling

Participant: Olivier Pantz.

Using a formal asymptotic expansion, we have proved with K. Trabelsi, that non-isotropic thin-structure could behave (when the thickness is small) like a shell combining both membrane and bending effects. It is the first time to our knowledge that such a model is derived. An article on this is currently under review.

6.4.4. A new Liouville type Rigidity Theorem

Participant: Olivier Pantz.

We have recently developed a new Liouville type Rigidity Theorem. Considering a cylindrical shaped solid, we prove that if the local area of the cross sections is preserved together with the length of the fibers, then the deformation is a combination of a planar deformation and a rigid motion. The results currently obtained are limited to regular deformations and we are currently working with B. Merlet to extend them. Nevertheless, we mainly focus on the case where the conditions imposed to the local area of the cross sections and the length of the fibers are only "almost" fulfilled. This will enable us to derive rigorously new non linear shell models combining both membrane and flexural effects that we have obtained using a formal approach.

6.5. Diffusion MRI

Participants: Jing-Rebecca Li, Houssem Haddar, Dang Van Nguyen, Hang Tuan Nguyen.

Diffusion Magnetic Resonance Imaging (DMRI) is a promising tool to obtain useful information on microscopic structure and has been extensively applied to biological tissues. In particular, we would like to focus on two applications:

- inferring from DMRI measurements changes in the cellular volume fraction occurring upon various physiological or pathological conditions.

  This application is one of the first to show the promise of DMRI because it can detect acute cerebral ischemia (cell swelling) on the basis of lower than normal apparent diffusion coefficient a few minutes after stroke.

- estimating the average cell size in the case of tumor imaging

  This application is useful as a diagnostic tool as well as a tool for the evaluation of tumor treatments.

For both of the above applications we approach the problem via the following steps:

- Construct reduced models of the multiple-compartment Bloch-Torrey partial differential equation (PDE) using homogenization methods.
- Invert the resulting reduced models for the biological parameters of interest: the cellular volume fraction in the first case, and the average distance between neighboring cells in the second case.

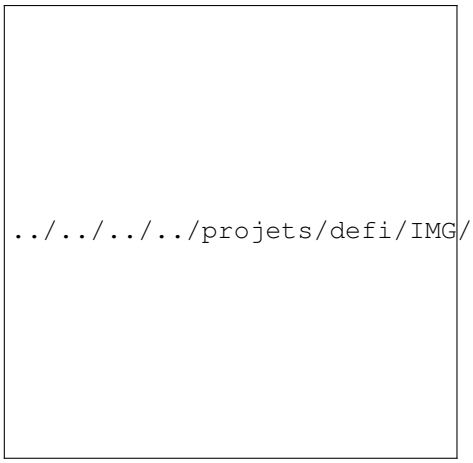


Figure 1. Computational domain for simulating diffusion in cerebral gray matter.

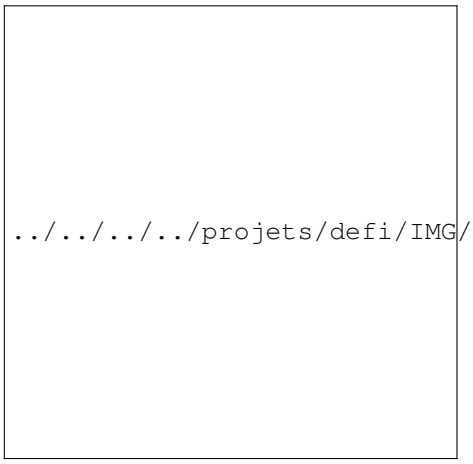


Figure 2. Computational domain for simulating tumor cells.

We obtained the following results.

- We generated fairly complicated meshes that can be used to simulate diffusion in cerebral gray matter. In the Finite Elements code, this required using the mesh generation software Salome, developed at the CEA Saclay. We are working on the problem of increasing the cellular volume fraction to a physically realistic level, which is difficult for the mesh generator because of the very small distances between the neurons. An article describing the Finite Elements code has been accepted by the Journal of Computational Physics, to be published in 2014. An article on a version of the code using Finite Volume discretization has been accepted by Physics in Medicine and Biology, published in 2013.
- We developed a reduce model of the DMRI signal using homogenization methods. Two articles on this topic have been submitted.

GAMMA3 Project-Team

4. New Results

4.1. From discrete to continuous metric fields

Participants: Patrick Laug [correspondant], Houman Borouchaki.

Adaptive computation using adaptive meshes is now recognized as essential for solving complex PDE problems. This computation requires at each step the definition of a continuous metric field to govern the generation of the adapted meshes. In practice, via an appropriate *a posteriori* error estimation, metrics are calculated at the vertices of the computational domain mesh. In order to obtain a continuous metric field, the discrete field is interpolated in the whole domain mesh. In this study, a new method for interpolating discrete metric fields, based on a so-called "natural decomposition" of metrics, is introduced. The proposed method is based on known matrix decompositions and is computationally robust and efficient. Some qualitative comparisons with classical methods are made to show the relevance of this methodology [19].

4.2. Hex-dominant meshing of geologic structures

Participants: Patrick Laug [correspondant], Houman Borouchaki.

Simulation by a finite volume method of the transfer by water of radioactive elements in sites of nuclear waste storage, on large time and space scales, is the only possible way to analyze the safety of disposal. To properly represent the different pathways of radionuclides, surface topography (valleys, reliefs, rivers), geologic layers and simplified storage facilities must be accurately modeled. We propose a new methodology for generating hex-dominant meshes (well suited for a finite volume formulation) of geologic structures complying with these different geometric constraints.

First, a reference 2D domain is obtained by projecting all the line constraints into a horizontal plane. Different size specifications are given for workings, outcrop lines and rivers. Using an adaptive methodology, the size variation is bounded by a specified threshold in order to obtain a high quality quad-dominant mesh. Secondly, a hex-dominant mesh of the geological medium is generated by a vertical extrusion. Depending on the configuration of the surfaces found (interfaces between two layers, top or bottom faces of underground workings), hexahedra, prisms, pyramids and tetrahedra are generated. The generation of volume elements follows a global order established on the whole set of surfaces to ensure the conformity of the resulting mesh. An example of mesh construction of a geologic structure illustrates the suitability of the proposed methodology [22].

4.3. Applications du maillage et développements de méthodes avancées pour la cryptographie

Participants: Thomas Grosges [correspondant], Dominique Barchiesi, Michael François
Validité du projet: 2009-2013.
Production scientifique: 1 thèse soutenue (M. François, 17/10/2012), 6 articles publiés.
L'utilisation des nombres (pseudo)-aléatoires a pris une dimension importante ces dernières décennies. De nombreuses applications dans le domaine des télécommunications, de la cryptographie, des simulations numériques ou encore des jeux de hasard, ont contribué au développement et à l'usage de ces nombres. Les méthodes utilisées pour la génération de tels nombres (pseudo)-aléatoires proviennent de deux types de processus : physique et algorithmique. Ce projet de recherche a donc pour objectif principal le développement de nouveaux procédés de génération de clés de chiffrement, dits "exotiques", basés sur des processus physiques, multi-échelles, multi-domaines assurant un niveau élevé de sécurité. Deux classes de générateurs basés sur des principes de mesures physiques et des processus mathématiques ont été développé.

La première classe de générateurs exploite la réponse d'un système physique servant de source pour la génération des séquences aléatoires. Cette classe utilise aussi bien des résultats de simulation que des résultats de mesures interférométriques pour produire des séquences de nombres aléatoires. L'application du maillage adaptatif sert au contrôle de l'erreur sur la solution des champs physiques (simulés ou mesurés). A partir de ces cartes physiques, un maillage avec estimateur d'erreur sur l'entropie du système est appliqué. Celui-ci permet de redistribuer les positions spatiales des noeuds. L'étude (locale) de la réduction d'entropie des clés tout au long de la chaîne de création et l'étude (globale) de l'entropie de l'espace des clés générées sont réalisées à partir de tests statistiques.

La seconde classe de générateurs porte sur le développement de méthodes avancées et est basée sur l'exploitation de fonctions chaotiques en utilisant les sorties de ces fonctions comme indice de permutation sur un vecteur initial. Ce projet s'intéresse également aux systèmes de chiffrement pour la protection des données et deux algorithmes de chiffrement d'images utilisant des fonctions chaotiques sont développés et analysés. Ces Algorithmes utilisent un processus de permutation-substitution sur les bits de l'image originale. Une analyse statistique approfondie confirme la pertinence des cryptosystèmes développés.

4.4. Développement de méthodes avancées et maillages appliqués à l'étude de la nanomorphologie des nanotubes/fils en suspension liquide"

Participants: Thomas Grosges [correspondant], Dominique Barchiesi, Abel Cherouat, Houman Borouchaki, Laurence Giraud-Moreau, Anis Chaari.
Validité du projet: 2011-2014.
Production scientifique: 1 thèse en cours (A. Chaari), 1 articles publiés, 1 conférence (CSMA 2013).
Ce projet de recherche (NANOMORPH) a pour objet principal le développement et la mise au point d'une instrumentation optique pour déterminer la distribution en tailles et le coefficient de forme de nanofils (NF) ou de nanotubes (NT) en suspension dans un écoulement. Au cours de ce projet, deux types de techniques optiques complémentaires sont développées. La première, basée sur la diffusion statique de la lumière, nécessite d'étudier au préalable la physico-chimie de la dispersion, la stabilisation et l'orientation des nanofils dans les milieux d'étude. La seconde méthode, basée sur une méthode opto-photothermique pulsée, nécessite en sus, la modélisation de l'interaction laser/nanofils, ainsi que l'étude des phénomènes multiphysiques induits par ce processus. L'implication de l'équipe-projet GAMMA3 concerne principalement la simulation multiphysique de l'interaction laser-nanofils et l'évolution temporelle des bulles et leurs formations. L'une des principales difficultés de ces problématiques est que la géométrie du domaine est variable (à la fois au sens géométrique et topologique). Ces simulations ne peuvent donc être réalisées que dans un schéma adaptatif de calcul nécessitant le remaillage tridimensionnel mobile, déformable avec topologie variable du domaine (formation et évolution des bulles au cours du temps et de l'espace).

4.5. Applications du maillage à des problèmes multi-physiques, développement de méthodes de résolutions avancées et modélisation électromagnetisme-thermique-mécanique à l'échelle mesoscopique

Participants: Dominique Barchiesi [correspondant], Abel Cherouat, Thomas Grosges, Houman Borouchaki, Laurence Giraud-Moreau, Sameh Kessentini, Anis Chaari, Fadhil Mezghani
Validité du projet: 2009-2015 (thèse de Fadhil Mezghani initiée en 2012 coencadrée par D. Barchiesi et A. Cherouat).
Production scientifique: 1 thèse soutenue (S. Kessentini, 22/10/2012), 9 articles publiés, 4 conférences.

Le contrôle et l'adaptation du maillage lors de la résolution de problèmes couplés ou/et non linéaires reste un problème ouvert et fortement dépendant du type de couplage physique entre les EDP à résoudre. Notre objectif est de développer des modèles stables afin de calculer les dilatations induites par l'absorption d'énergie électromagnétique, par des structures matérielles inférieures au micron. Les structures étudiées sont en particulier des nanoparticules métalliques en condition de résonance plasmon. Dans ce cas, un maximum d'énergie absorbée est attendu, accompagné d'un maximum d'élévation de température et de dilatation. Il faut en particulier développer des modèles permettant de simuler le comportement multiphysique de particules de formes quelconques, pour une gamme de fréquences du laser d'éclairage assez étendue afin d'obtenir une étude spectroscopique de la température et de la dilatation. L'objectif intermédiaire est de pouvoir quantifier la dilatation en fonction de la puissance laser incidente. Le calcul doit donc être dimensionné et permettre finalement des applications dans les domaines des capteurs et de l'ingénierie biomédicale. En effet, ces nanoparticules métalliques sont utilisées à la fois pour le traitement des cancers superficiels par nécrose de tumeur sous éclairage adéquat, dans la fenêtres de transparence cellulaire. Déposées sur un substrat de verre, ces nanoparticules permettent de construire des capteurs utilisant la résonance plasmon pour être plus sensibles (voir projet européen *Nanoantenna* et l'activité génération de nombres aléatoires). Cependant, dans les deux cas, il est nécessaire, en environnement complexe de déterminer la température locale, voire la dilatation de ces nanoparticules, pouvant conduire à un désaccord du capteur, la résonance plasmon étant très sensible aux paramètres géométriques et matériels des nanostructures. Dans ce sens, l'étude permet d'aller plus loin que la << simple >> interaction électromagnétique avec la matière du projet européen *Nanoantenna*.

Le travail de l'année 2013 a constitué en la poursuite de la pré-étude des spécificités de ce type de problème multiphysique pour des structures de forme simple et la mise en place de fonctions test, de référence, pour les développements de maillage adaptatifs pour les modèles multiphysiques éléments finis. Nous espérons pouvoir proposer un projet ANR couplant les points de vue microscopiques et macroscopiques dans les deux années qui viennent.

4.6. Validity of rational and nonrational Lagrange finite elements of degree 1 and 2

Participants: Paul-Louis George [correspondant], Houman Borouchaki.

A finite element is valid if its jacobian is strictly positive everywhere. The jacobian is the determinant of the jacobian matrix related to the partials of the mapping function which maps the parameter space (reference element) to the current element. Apart when it is constant, the jacobian is a polynomial whose degree is related to the degree of the finite element (but not the same in general). The value of the jacobian varies after the point where it is evaluated. Validating an element relies in finding the sign of this polynomial when one traverses the element.

Various papesr and a synthesis of those reports, shows how to calculating the jacobian of the different usual Lagrange finite elements of degree 1 and 2. To this end, we take the form of this polynomial as obtained in the classical finite element framework (shape functions and nodes) or after reformulating the element by means of a Bezier form (Bernstein polynomials and control points) which makes easier the discussion. We exhibit sufficient (necessary and sufficient in some cases) conditions to ensure the validity of a given element.

4.7. Mesh adaptation for very high-order numerical scheme

Participants: Frédéric Alauzet [correspondant], Adrien Loseille, Estelle Mbinky.

In the past, we have demonstrated that multi-scale anisotropic mesh adaptation is a powerful tool to accurately simulate compressible flow problems and to obtain faster convergence to continuous solutions. But, this was limited to second order numerical scheme. Nowadays, numerous teams are working on the development of very high-order numerical scheme (e.g. of third or greater order): Discontinous Galerkin, Residual Distribution scheme, Spectral method, ...

This work extend interpolation error estimates to higher order numerical solution representation. We have examined the case of third-order accuracy. The first step is to reduce the tri-linear form given by the third order error term into a quadratic form based on the third order derivative. From this local error model, the optimal mesh is exhibited thanks to the continuous mesh framework.

4.8. Visualization and modification of high-order curved meshes

Participants: Julien Castelneau, Adrien Loseille [correspondant], Loïc Maréchal.

During the partnership between Inria and Distene, a new visualization software has been designed. It address the typical operations that are required to quickly assess the newly algorithm developed in the team. In particular, interactive modifications of high-order curved mesh has been addressed. The software VIZIR is freely available at https://www.rocq.inria.fr/gamma/gamma/vizir/.

4.9. A changing-topology ALE numerical scheme

Participants: Frédéric Alauzet [correspondant], Nicolas Barral.

The main difficulty arising in numerical simulations with moving geometries is to handle the displacement of the domain boundaries, *i.e.,* the moving bodies. Only vertices displacement is not sufficient to achieve complex movement such as shear. We proved that the use of edge swapping allows us to achieve such complex displacement. We therefore developed an ALE formulation of this topological mesh modification to preserve the solver accuracy and convergence order. The goal is to extend to 3D the previous work done in 2D.

4.10. Mesh adaptation for Navier-Stokes Equations

Participants: Frédéric Alauzet, Victorien Menier, Adrien Loseille [correspondant].

Adaptive simulations for Navier-Stokes equations require to propose accurate error estimates and design robust mesh adaptation algorithms (for boundary layers).

For error estimates, we design new estimates suited to accurately capture the speed profile in the boundary layers. For mesh adaptation, we design a new method to generate structured boundary layer meshes which are mandatory to accurately compute compressible flows a high Reynolds number (several millions). It couple the specification of the optimal boundary layer from the geometry boundary and moving mesh techniques to extrude the boundary layer in an already existing mesh. The main advantage of this approach is its robustness, *i.e.,* at each step of the algorithm we have always a valid mesh.

4.11. Serial and parallel cavity-based mesh adaptation

Participants: Victorien Menier, Adrien Loseille [correspondant].

A new algorithm to derive adaptive meshes has been introduced through new cavity-based algorithms. It allows to generate anisotropic surface and volume mesh along with adaptive quasi-structured elements. The later point is of main interest when dealing with viscous phenomena where a boundary layer mesh is needed [26].

In addition, a parallel version of the algorithm was designed [27].

IPSO Project-Team

5. New Results

5.1. Multi-revolution composition methods for highly oscillatory differential equations

In [45], we introduce a new class of multi-revolution composition methods (MRCM) for the approximation of the Nth-iterate of a given near-identity map. When applied to the numerical integration of highly oscillatory systems of differential equations, the technique benefits from the properties of standard composition methods: it is intrinsically geometric and well-suited for Hamiltonian or divergence-free equations for instance. We prove error estimates with error constants that are independent of the oscillatory frequency. Numerical experiments, in particular for the nonlinear Schrödinger equation, illustrate the theoretical results, as well as the efficiency and versatility of the methods.

5.2. Weak second order multi-revolution composition methods for highly oscillatory stochastic differential equations with additive or multiplicative noise

In [61], we introduce a class of numerical methods for highly oscillatory systems of stochastic differential equations with general noncommutative noise. We prove global weak error bounds of order two uniformly with respect to the stiffness of the oscillations, which permits to use large time steps. The approach is based on the micro-macro framework of multi-revolution composition methods recently introduced for deterministic problems and inherits its geometric features, in particular to design integrators preserving exactly quadratic first integral. Numerical experiments, including the stochastic nonlinear Schrödinger equation with space-time multiplicative noise, illustrate the performance and versatility of the approach.

5.3. High order numerical approximation of the invariant measure of ergodic SDEs

In [41], we introduce new sufficient conditions for a numerical method to approximate with high order of accuracy the invariant measure of an ergodic system of stochastic differential equations, independently of the weak order of accuracy of the method. We then present a systematic procedure based on the framework of modified differential equations for the construction of stochastic integrators that capture the invariant measure of a wide class of ergodic SDEs (Brownian and Langevin dynamics) with an accuracy independent of the weak order of the underlying method. Numerical experiments confirm our theoretical findings.

5.4. PIROCK: a swiss-knife partitioned implicit-explicit orthogonal Runge-Kutta Chebyshev integrator for stiff diffusion-advection-reaction problems with or without noise

In [13], a partitioned implicit-explicit orthogonal Runge-Kutta method (PIROCK) is proposed for the time integration of diffusion-advection-reaction problems with possibly severely stiff reaction terms and stiff stochastic terms. The diffusion terms are solved by the explicit second order orthogonal Chebyshev method (ROCK2), while the stiff reaction terms (solved implicitly) and the advection and noise terms (solved explicitly) are integrated in the algorithm as finishing procedures. It is shown that the various coupling (between diffusion, reaction, advection and noise) can be stabilized in the PIROCK method. The method, implemented in a single black-box code that is fully adaptive, provides error estimators for the various terms present in the problem, and requires from the user solely the right-hand side of the differential equation. Numerical experiments and comparisons with existing Chebyshev methods, IMEX methods and partitioned methods show the efficiency and flexibility of our new algorithm.

5.5. An offline-online homogenization strategy to solve quasilinear two-scale problems at the cost of one-scale problems

In [39], inspired by recent analyses of the finite element heterogeneous multiscale method and the reduced basis technique for nonlinear problems, we present a simple and concise finite element algorithm for the reliable and efficient resolution of elliptic or parabolic multiscale problems of nonmonotone type. Solutions of appropriate cell problems on sampling domains are selected by a greedy algorithm in an offline stage and assembled in a reduced basis (RB). This RB is then used in an online stage to solve two-scale problems at a computational cost comparable to the single-scale case. Both the offline and the online cost are independent of the smallest scale in the physical problem. The performance and accuracy of the algorithm are illustrated on 2D and 3D stationary and evolutionary nonlinear multiscale problems.

5.6. Reduced basis finite element heterogeneous multiscale method for quasilinear elliptic homogenization problems

In [40], a reduced basis nite element heterogeneous multiscale method (RB-FE-HMM) for a class of nonlinear homogenization elliptic problems of nonmonotone type is introduced. In this approach, the solutions of the micro problems needed to estimate the macroscopic data of the homogenized problem are selected by a Greedy algorithm and computed in an online stage. It is shown that the use of reduced basis (RB) for nonlinear numerical homogenization reduces considerably the computational cost of the nite element heterogeneous multiscale method (FE-HMM). As the precomputed microscopic functions depend nonlinearly on the macroscopic solution, we introduce a new a posteriori error estimator for the Greedy algorithm that guarantees the convergence of the online Newton method. A priori error estimates and uniqueness of the numerical solution are also established. Numerical experiments illustrate the e ciency of the proposed method.

5.7. Weak second order explicit stabilized methods for stiff stochastic differential equations

In [16], we introduce a new family of explicit integrators for stiff Itô stochastic differential equations (SDEs) of weak order two. These numerical methods belong to the class of one-step stabilized methods with extended stability domains and do not suffer from the stepsize reduction faced by standard explicit methods. The family is based on the standard second order orthogonal Runge-Kutta Chebyshev methods (ROCK2) for deterministic problems. The convergence, and the mean-square and asymptotic stability properties of the methods are analyzed. Numerical experiments, including applications to nonlinear SDEs and parabolic stochastic partial differential equations are presented and confirm the theoretical results.

5.8. Mean-square A-stable diagonally drift-implicit integrators of weak second order for stiff Itô stochastic differential equations

In [15], we introduce two drift-diagonally-implicit and derivative-free integrators for stiff systems of Itô stochastic differential equations with general non-commutative noise which have weak order 2 and deterministic order 2, 3, respectively. The methods are shown to be mean-square A-stable for the usual complex scalar linear test problem with multiplicative noise and improve significantly the stability properties of the drift-diagonally-implicit methods previously introduced [K. Debrabant and A. Rößler, Appl. Num. Math., 59, 2009].

5.9. Two-Scale Macro-Micro decomposition of the Vlasov equation with a strong magnetic field

In [25], we build a Two-Scale Macro-Micro decomposition of the Vlasov equation with a strong magnetic field. This consists in writing the solution of this equation as a sum of two oscillating functions with circonscribed oscillations. The first of these functions has a shape which is close to the shape of the Two-Scale limit of the solution and the second one is a correction built to offset this imposed shape. The aim of such a decomposition is to be the starting point for the construction of Two-Scale Asymptotic-Preserving Schemes.

5.10. A dynamic multi-scale model for transient radiative transfer calculations

In [33], a dynamic multi-scale model which couples the transient radiative transfer equation (RTE) and the diffusion equation (DE) is proposed and validated. It is based on a domain decomposition method where the system is divided into a mesoscopic subdomain, where the RTE is solved, and a macroscopic subdomain where the DE is solved. A buffer zone is introduced between the mesoscopic and the macroscopic subdomains, as proposed by Degond and Jin, who solve a coupled system of two equations, one at the mesoscopic and the other at the macroscopic scale. The DE and the RTE are coupled through the equations inside the buffer zone, instead of being coupled through a geometric interface like in standard domain decomposition methods. One main advantage is that no boundary or interface conditions are needed for the DE. The model is compared to Monte Carlo, finite volume and P1 solutions in one dimensional stationary and transient test cases, and presents promising results in terms of trade-off between accuracy and computational requirements.

5.11. Quasi-periodic solutions of the 2D Euler equation

In [24], we consider the two-dimensional Euler equation with periodic boundary conditions. We construct time quasi-periodic solutions of this equation made of localized travelling profiles with compact support propagating over a stationary state depending on only one variable. The direction of propagation is orthogonal to this variable, and the support is concentrated on flat strips of the stationary state. The frequencies of the solution are given by the locally constant velocities associated with the stationary state.

5.12. Optimization and parallelization of Emedge3D on shared memory architecture

In [38], a study of techniques used to speedup a scientific simulation code is presented. The techniques include sequential optimizations as well as the parallelization with OpenMP. This work is carried out on two different multicore shared memory architectures, namely a cutting edge 8x8 core CPU and a more common 2x6 core board. Our target application is representative of many memory bound codes, and the techniques we present show how to overcome the burden of the memory bandwidth limit, which is quickly reached on multi-core or many-core with shared memory architectures. To achieve efficient speedups, strategies are applied to lower the computation costs, and to maximize the use of processors caches. Optimizations are: minimizing memory accesses, simplifying and reordering computations, and tiling loops. On 12 cores processor Intel X5675, aggregation of these optimizations results in an execution time 21.6 faster, compared to the original version on one core.

5.13. Vlasov on GPU (VOG Project)

In [58], we are concerned with the numerical simulation of the Vlasov-Poisson set of equations using semi- Lagrangian methods on Graphical Processing Units (GPU). To accomplish this goal, modifications to traditional methods had to be implemented. First and foremost, a reformulation of semi-Lagrangian methods is performed, which enables us to rewrite the governing equations as a circulant matrix operating on the vector of unknowns. This product calculation can be performed efficiently using FFT routines. Second, to overcome the limitation of single precision inherent in GPU, a δf type method is adopted which only needs refinement in specialized areas of phase space but not throughout. Thus, a GPU Vlasov-Poisson solver can indeed perform high precision simulations (since it uses very high order reconstruction methods and a large number of grid points in phase space). We show results for rather academic test cases on Landau damping and also for physically relevant phenomena such as the bump on tail instability and the simulation of Kinetic Electrostatic Electron Nonlinear (KEEN) waves.

5.14. Uniformly accurate numerical schemes for highly oscillatory Klein-Gordon and nonlinear Schrödinger equations

In [37], we are interested in the numerical simulation of nonlinear Schrödinger and Klein-Gordon equations. We present a general strategy to construct numerical schemes which are uniformly accurate with respect to the oscillation frequency. This is a stronger feature than the usual so called "Asymptotic preserving" property, the last being also satisfied by our scheme in the highly oscillatory limit. Our strategy enables to simulate the oscillatory problem without using any mesh or time step refinement, and the orders of our schemes are preserved uniformly in all regimes. In other words, since our numerical method is not based on the derivation and the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, in the highly oscillatory limit regime, and in the intermediate regime with the same order of accuracy. The method is based on two main ingredients. First, we embed our problem in a suitable "two-scale" reformulation with the introduction of an additional variable. Then a link is made with classical strategies based on Chapman-Enskog expansions in kinetic theory despite the dispersive context of the targeted equations, allowing to separate the fast time scale from the slow one. Uniformly accurate (UA) schemes are eventually derived from this new formulation and their properties and performances are assessed both theoretically and numerically.

5.15. Asymptotic preserving schemes for the Wigner-Poisson-BGK equations in the diffusion limit

In [26], we focus on the numerical simulation of the Wigner-Poisson-BGK equation in the diffusion asymptotics. Our strategy is based on a "micro-macro" decomposition, which leads to a system of equations that couple the macroscopic evolution (diffusion) to a microscopic kinetic contribution for the fluctuations. A semi-implicit discretization provides a numerical scheme which is stable with respect to the small parameter ε (mean free path) and which possesses the following properties: (i) it enjoys the asymptotic preserving property in the diffusive limit; (ii) it recovers a standard discretization of the Wigner-Poisson equation in the collisionless regime. Numerical experiments confirm the good behaviour of the numerical scheme in both regimes. The case of a spatially dependent $\varepsilon(x)$ is also investigated.

5.16. Existence and stability of solitons for fully discrete approximations of the nonlinear Schrödinger equation

In [19], we study the long time behavior of a discrete approximation in time and space of the cubic nonlinear Schrödinger equation on the real line. More precisely, we consider a symplectic time splitting integrator applied to a discrete nonlinear Schrödinger equation with additional Dirichlet boundary conditions on a large interval. We give conditions ensuring the existence of a numerical soliton which is close in energy norm to the continuous soliton. Such result is valid under a CFL condition between the time and space stepsizes. Furthermore we prove that if the initial datum is symmetric and close to the continuous soliton, then the associated numerical solution remains close to the orbit of the continuous soliton for very long times.

5.17. Asymptotic preserving schemes for the Klein-Gordon equation in the non-relativistic limit regime

In [32], we consider the Klein-Gordon equation in the non-relativistic limit regime, i.e. the speed of light c tending to infinity. We construct an asymptotic expansion for the solution with respect to the small parameter depending on the inverse of the square of the speed of light. As the first terms of this asymptotic can easily be simulated our approach allows us to construct numerical algorithms that are robust with respect to the large parameter c producing high oscillations in the exact solution.

5.18. Sobolev stability of plane wave solutions to the cubic nonlinear Schrödinger equation on a torus

In [31], it is shown that plane wave solutions to the cubic nonlinear Schrödinger equation on a torus behave orbitally stable under generic perturbations of the initial data that are small in a high-order Sobolev norm, over long times that extend to arbitrary negative powers of the smallness parameter. The perturbation stays small in the same Sobolev norm over such long times. The proof uses a Hamiltonian reduction and transformation and, alternatively, Birkhoff normal forms or modulated Fourier expansions in time.

5.19. Weak backward error analysis for overdamped Langevin equation

In [57], we consider an overdamped Langevin stochastic differential equation and show a weak backward error analysis result for its numerical approximations defined by implicit methods. In particular, we prove that the generator associated with the numerical solution coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the stepsize. This implies that every measure of the numerical scheme is close to a modified invariant measure obtained by asymptotic expansion. Moreover, we prove that, up to negligible terms, the dynamic associated with the implicit scheme considered is exponentially mixing.

5.20. Weak backward error analysis for Langevin equation

In [56], We consider numerical approximations of stochastic Langevin equations by implicit methods. We show a weak backward error analysis result in the sense that the generator associated with the numerical solution coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the stepsize. This implies that every measure of the numerical scheme is close to a modified invariant measure obtained by asymptotic expansion. Moreover, we prove that, up to negligible terms, the dynamic associated with the implicit scheme considered is exponentially mixing.

5.21. Approximation of the invariant law of SPDEs: error analysis using a Poisson equation for a full-discretization scheme

In [44], we study the long-time behavior of fully discretized semilinear SPDEs with additive space-time white noise, which admit a unique invariant probability measure μ. We show that the average of regular enough test functions with respect to the (possibly non unique) invariant laws of the approximations are close to the corresponding quantity for μ.

More precisely, we analyze the rate of the convergence with respect to the different discretization parameters. Here we focus on the discretization in time thanks to a scheme of Euler type, and on a Finite Element discretization in space.

The results rely on the use of a Poisson equation; we obtain that the rates of convergence for the invariant laws are given by the weak order of the discretization on finite time intervals: order $1/2$ with respect to the time-step and order 1 with respect to the mesh-size.

5.22. An asymptotic preserving scheme based on a new formulation for NLS in the semiclassical limit

In [20], we consider the semiclassical limit for the nonlinear Schrodinger equation. We introduce a phase/amplitude representation given by a system similar to the hydrodynamical formulation, whose novelty consists in including some asymptotically vanishing viscosity. We prove that the system is always locally well-posed in a class of Sobolev spaces, and globally well-posed for a fixed positive Planck constant in the one-dimensional case. We propose a second order numerical scheme which is asymptotic preserving. Before singularities appear in the limiting Euler equation, we recover the quadratic physical observables as well as the wave function with mesh size and time step independent of the Planck constant. This approach is also well suited to the linear Schrodinger equation.

5.23. Asymptotic Preserving schemes for highly oscillatory Vlasov-Poisson equations

The work [28] is devoted to the numerical simulation of a Vlasov-Poisson model describing a charged particle beam under the action of a rapidly oscillating external field. We construct an Asymptotic Preserving numerical scheme for this kinetic equation in the highly oscillatory limit. This scheme enables to simulate the problem without using any time step refinement technique. Moreover, since our numerical method is not based on the derivation of the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, and in the highly oscillatory regime as well. Our method is based on a "two scale" reformulation of the initial equation, with the introduction of an additional periodic variable.

5.24. Uniformly accurate numerical schemes for highly oscillatory Klein-Gordon and nonlinear Schrödinger equations

The work [37] is devoted to the numerical simulation of nonlinear Schrödinger and Klein-Gordon equations. We present a general strategy to construct numerical schemes which are uniformly accurate with respect to the oscillation frequency. This is a stronger feature than the usual so called ”Asymptotic preserving" property, the last being also satisfied by our scheme in the highly oscillatory limit. Our strategy enables to simulate the oscillatory problem without using any mesh or time step refinement, and the orders of our schemes are preserved uniformly in all regimes. In other words, since our numerical method is not based on the derivation and the simulation of asymptotic models, it works in the regime where the solution does not oscillate rapidly, in the highly oscillatory limit regime, and in the intermediate regime with the same order of accuracy. In the same spirit as in [28], the method is based on two main ingredients. First, we embed our problem in a suitable ”two-scale" reformulation with the introduction of an additional variable. Then a link is made with classical strategies based on Chapman-Enskog expansions in kinetic theory despite the dispersive context of the targeted equations, allowing to separate the fast time scale from the slow one. Uniformly accurate (UA) schemes are eventually derived from this new formulation and their properties and performances are assessed both theoretically and numerically.

5.25. On the controllability of quantum transport in an electronic nanostructure

In [59], we investigate the controllability of quantum electrons trapped in a two-dimensional device, typically a MOS field-effect transistor. The problem is modeled by the Schrödinger equation in a bounded domain coupled to the Poisson equation for the electrical potential. The controller acts on the system through the boundary condition on the potential, on a part of the boundary modeling the gate. We prove that, generically with respect to the shape of the domain and boundary conditions on the gate, the device is controllable. We also consider control properties of a more realistic nonlinear version of the device, taking into account the self-consistent electrostatic Poisson potential.

5.26. The Interaction Picture method for solving the generalized nonlinear Schrödinger equation in optics

The ”interaction picture” (IP) method is a very promising alternative to Split-Step methods for solving certain type of partial differential equations such as the nonlinear Schrödinger equation involved in the simulation of wave propagation in optical fibers. The method exhibits interesting convergence properties and is likely to provide more accurate numerical results than cost comparable Split-Step methods such as the Symmetric Split-Step method. In [42] we investigate in detail the numerical properties of the IP method and carry out a precise comparison between the IP method and the Symmetric Split-Step method.

5.27. Solving highly-oscillatory NLS with SAM: numerical efficiency and geometric properties

In [46], we present the Stroboscopic Averaging Method (SAM), recently introduced in [7,8,10,12], which aims at numerically solving highly-oscillatory differential equations. More specifically, we first apply SAM to the Schrödinger equation on the 1-dimensional torus and on the real line with harmonic potential, with the aim of assessing its efficiency: as compared to the well-established standard splitting schemes, the stiffer the problem is, the larger the speed-up grows (up to a factor 100 in our tests). The geometric properties of SAM are also explored: on very long time intervals, symmetric implementations of the method show a very good preservation of the mass invariant and of the energy. In a second series of experiments on 2-dimensional equations, we demonstrate the ability of SAM to capture qualitatively the long-time evolution of the solution (without spurring high oscillations).

5.28. Analysis of models for quantum transport of electrons in graphene layers

In [51], we present and analyze two mathematical models for the self consistent quantum transport of electrons in a graphene layer. We treat two situations. First, when the particles can move in all the plane R^2, the model takes the form of a system of massless Dirac equations coupled together by a selfconsistent potential, which is the trace in the plane of the graphene of the 3D Poisson potential associated to surface densities. In this case, we prove local in time existence and uniqueness of a solution in $H^s(R^2)$, for $s > 3/8$ which includes in particular the energy space $H^{1/2}(R^2)$. The main tools that enable to reach $s \in (3/8, 1/2)$ are the dispersive Strichartz estimates that we generalized here for mixed quantum states. Second, we consider a situation where the particles are constrained in a regular bounded domain Ω. In order to take into account Dirichlet boundary conditions which are not compatible with the Dirac Hamiltonian H_0, we propose a different model built on a modified Hamiltonian displaying the same energy band diagram as H_0 near the Dirac points. The well-posedness of the system in this case is proved in H^s_A, the domain of the fractional order Dirichlet Laplacian operator, for $1/2 \leq s$.

5.29. Analysis of a large number of Markov chains competing for transitions

In [18], we consider the behavior of a stochastic system composed of several identically distributed, but non independent, discrete-time absorbing Markov chains competing at each instant for a transition. The competition consists in determining at each instant, using a given probability distribution, the only Markov chain allowed to make a transition. We analyze the first time at which one of the Markov chains reaches its absorbing state. When the number of Markov chains goes to infinity, we analyze the asymptotic behavior of the system for an arbitrary probability mass function governing the competition. We give conditions for the existence of the asymptotic distribution and we show how these results apply to cluster-based distributed systems when the competition between the Markov chains is handled by using a geometric distribution.

5.30. Markov Chains Competing for Transitions: Application to Large-Scale Distributed Systems

In [17], we consider the behavior of a stochastic system composed of several identically distributed, but non independent, discrete-time absorbing Markov chains competing at each instant for a transition. The competition consists in determining at each instant, using a given probability distribution, the only Markov chain allowed to make a transition. We analyze the first time at which one of the Markov chains reaches its absorbing state. We obtain its distribution and its expectation and we propose an algorithm to compute these quantities. We also exhibit the asymptotic behavior of the system when the number of Markov chains goes to infinity. Actually, this problem comes from the analysis of large-scale distributed systems and we show how our results apply to this domain.

5.31. Existence of densities for the 3D Navier–Stokes equations driven by Gaussian noise

In [30], we prove three results on the existence of densities for the laws of finite dimensional functionals of the solutions of the stochastic Navier-Stokes equations in dimension 3. In particular, under very mild assumptions on the noise, we prove that finite dimensional projections of the solutions have densi- ties with respect to the Lebesgue measure which have some smoothness when measured in a Besov space. This is proved thanks to a new argument inspired by an idea introduced by N. Fournier and J. Printems.

5.32. Invariant measure of scalar first-order conservation laws with stochastic forcing

In [50], we assume an hypothesis of non-degeneracy of the flux and study the long-time behaviour of periodic scalar first-order conservation laws with stochastic forcing in any space dimension. For sub-cubic fluxes, we show the existence of an invariant measure. Moreover for sub-quadratic fluxes we show uniqueness and ergodicity of the invariant measure. Also, since this invariant measure is supported by L^p for some p small, we are led to generalize to the stochastic case the theory of L^1 solutions developed by Chen and Perthame.

5.33. Degenerate Parabolic Stochastic Partial Differential Equations: Quasilinear case

In [49], we study the Cauchy problem for a quasilinear degenerate parabolic stochastic partial differential equation driven by a cylindrical Wiener process. In particular, we adapt the notion of kinetic formulation and kinetic solution and develop a well-posedness theory that includes also an L^1-contraction property. In comparison to the previous works of the authors concerning stochastic hyperbolic conservation laws and semilinear degenerate parabolic SPDEs, the present result contains two new ingredients that provide simpler and more effective method of the proof: a generalized Itô formula that permits a rigorous derivation of the kinetic formulation even in the case of weak solutions of certain nondegenerate approximations and a direct proof of strong convergence of these approximations to the desired kinetic solution of the degenerate problem.

5.34. Existence of densities for stable-like driven SDE's with Hölder continuous coefficients

In [29], we consider a multidimensional stochastic differential equation driven by a stable-like Lévy process. We prove that the law of the solution immediately has a density in some Besov space, under some non-degeneracy condition on the driving Lévy process and some very light Hölder-continuity assumptions on the drift and diffusion coefficients.

5.35. Ergodicity results for the stochastic Navier-Stokes equations: an introduction

In the chapter [36], we give an overview of the results on ergodicity for the stochastic Navier-Stokes equations. We first explain the basis on SPDEs and on the concept of invariant measures and ergodicity. Then, in the 2D case, we introduce progressively the various methods, finishing with a celebrated result due to M. Hairer and J. Mattingly on ergodicity with very degenerated noises. In the 3D case, the theory is much less complete. Nonetheles, we show that it is possible to construct Markov evolutions and, under some non degenary assumptions on the noise, to obtain ergodicity.

5.36. Weak truncation error estimates for elliptic PDEs with lognormal coefficients

In [22], we are interested in the weak error committed on the solution of an elliptic partial differential equation with a lognormal coefficient, resulting from the approximation of the lognormal coefficient through a Karhunen-Loéve expansion. We improve results of a previous work, in which L^p-estimates of the weak error are provided. Only small enough values of p (the corresponding values of p depend on the space dimension) could be considered and such bounds are not sufficient to be applied to practical cases. Moreover, the optimality of this weak order (which turns out to be twice the strong order) has not been studied numerically. Therefore, the aim of this paper is double. First we improve drastically the weak error estimate by providing a bound of the C^1-norm of the weak error. This requires regularity results in Hölder spaces, with explicit bounds for the constants. We also consider much more general test functions in the definition of the weak error. Finally, we show the optimality of the weak order and illustrate this weak convergence with numerical results.

5.37. Optimized high-order splitting methods for some classes of parabolic equations

In [21], we are concerned with the numerical solution obtained by splitting methods of certain parabolic partial differential equations. Splitting schemes of order higher than two with real coefficients necessarily involve negative coefficients. It has been demonstrated that this second-order barrier can be overcome by using splitting methods with complex-valued coefficients (with positive real parts). In this way, methods of orders 3 to 14 by using the Suzuki-Yoshida triple (and quadruple) jump composition procedure have been explicitly built. Here we reconsider this technique and show that it is inherently bounded to order 14 and clearly sub-optimal with respect to error constants. As an alternative, we solve directly the algebraic equations arising from the order conditions and construct methods of orders 6 and 8 that are the most accurate ones available at present time, even when low accuracies are desired. We also show that, in the general case, 14 is not an order barrier for splitting methods with complex coefficients with positive real part by building explicitly a method of order 16 as a composition of methods of order 8.

5.38. Higher-Order Averaging, Formal Series and Numerical Integration III: Error Bounds

In earlier papers, it has been shown how formal series like those used nowadays to investigate the properties of numerical integrators may be used to construct high-order averaged systems or formal first integrals of Hamiltonian problems. With the new approach the averaged system (or the formal first integral) may be written down immediately in terms of (i) suitable basis functions and (ii) scalar coefficients that are computed via simple recursions. In [23], we show how the coefficients/basis functions approach may be used advantageously to derive exponentially small error bounds for averaged systems and approximate first integrals.

MC2 Project-Team

6. New Results

6.1. Cancer modelling

We have improved our generic mathematical models describing tumor growth. These models were then specialized for several types of cancer (thyroidal lung nodules, brain tumors). The algorithm used to recover the parameters of these models from medical images has also been greatly improved and is now adapted to run on HPC architectures.

- Secondary tumors in the lung:
  The mathematical models describing the growth of secondary in the lungs have now settled and are well understood. The main focus of the year was to keep on using these models on patient data. New clinical case were selected by clinicians from the Institut Bergonié, there are currently under study. The model is currently able to reproduce the growth observed on 5 clinical cases. Huge improvements to the calibration algorithms were made. The initial seeding of the algorithms was a weak point of the procedure and the robustness regarding the time-derivative of the observations is now much more accurate. A complete rewrite of the routines was done to improve their versatility and efficiency. Previously, the numerical simulations and calibration were performed in 2D (clinicians selected the most relevant slice showing the evolution of the tumor). Work is now ongoing to switch to full 3D computations and calibration. A newly hired engineer is testing our calibration technique on a dozen of clinical cases.
- Metastasis to the liver of a GIST
  We have derived a continuous model describing the growth of a GIST metastasis to the liver treated with Glivec and Sutent. This model is able to qualitatively reproduce the evolution observed on two different patients. Work has also started on developing new markers computed from the texture of the tumor seen on images to be able to detect any change in the response to treatment. This was the subject of an internship in the General Electric Healthcare research center. The results are promising so far.
- Modeling glioblastomas:
  In 2011, a hierarchy of models describing the growth of brain tumors was developed (and described in a submitted paper) in collaboration with University of Alabama at Birmingham. As we wished to obtain models that could be calibrated from patient data and yet be reasonably accurate, we believe that these models are suitable trade-offs between the simplicity of the Swanson's model (the only one used on patient data of brain tumors so far) and the accuracy of more complex models (that cannot really produce quantitative results). We have derived a new model that allows us to study the efficency of anti-angiogenic therapies. It seems to predict that the efficacy of these treatments is limited, this could be confirmed by a world-wide ongoing clinical study. Work is ongoing with this model to develop new marker to quantify patient anti-angiogenic drugs as soon as possible. This collaboration will be made stronger by a new Phd in UAB co-advised by T. Colin.
- Modelling of electrochemotherapy :
  Two articles related to the electrical cell modelling have been done ([59], [56]) . The first one deals with the influence of the ionic fluxes on the transmembrane voltage potential and on the cell volume. The main insight of the results consists in linking the transmembrane potential with the cell volume: it has been observed experimentally that cells with a low voltage potential do divide, whereas cells with high voltage potential do not, and the obtained relationship between voltage potential and cell volume can provide an explanation. The second article deals with a new model of cell electroporation essentially based on the experimental results of the I.G.R. In this paper we describe precisely the model, which takes into account the main experimental results in the electroporation process, and we present a variationnal formulation inherent to the model that leads to new efficient schemes in order to numerically solve the involved P.D.E.

The article describing a new electrical model of classical has been published in Journal of Math Biology. This new phenomenological model involves much less parameters than the usual models, but it still provides the qualitatively good description of the electroporation. The main feature of this model lies in the fact that it provides an intrinsic behavior of the cell membrane, which seems in accordance with the preliminary experimental results of the IGR partner. We also adapted the finite difference method developed by L. Weynans and M. Cisternino for elliptic interface problems to the electropermeabilization model developed recently by C. Poignard with O. Kavian. The new method has been validated by convergence tests and comparison with other models. We have proven that in one dimension the numerical solution converges to the solution of the exact problem. A paper describing these results has been submitted. A second-order Cartesian method for the simulation of electropermeabilization cell models, Leguebe M., Poignard C., Weynans L., Inria Resaerch Report RR-8302).

- Cell Migration modelling:
  The collaboration with IECB (University of Bordeaux) has continued with the postdocatoral position of Julie Joie. We have obtain a continuous model of cell density evolving on micropatterned polymers. The research report RR 7998 will be published in Math. Biosci. and Eng. A discrete model describing the single cells motility is being written.

  We also have started a collaboration with the University of Osaka (Japan), thanks to a PHC Sakura project, on the invadopodia. C. Poignard has been invited at Osaka in february by Prof. Suzuki. A model describing the destruction of the extracellular matrix by the MMP enzyme, and then the cell migration has been obtained. R. Mahumet, a PhD student of Prof. Suzuki is developing a code to simulate the model.
- Adaptive radiotherapy: a new work is also ongoing with Institut Bergonié to quantify the movement and deformations of organs of patients with sarcoma treated with radiotherapy. The preliminary results highlight that these mouvements are much larger than clinicians expected. We are now working on improving our workflow and developing a new segmentation technique to have this monitoring automatically performed (for the time being clinicians have to delineate each structure which is a very time consuming task). The ultimate goal is to change the therapeutical protocol to take these movements into account (which is currently not the case). Preliminary contacts have been made with a company developing a dose computing software to evaluate the efficacy of an adaptive planning of the Radio-Therapy compared to the constant dose plan currently given to the patient.
- Modeling meningioma growth and their responses to radiotherapy: In collaboration with Institut Bergonié, we have started developing new models for studying meningioma. Our model is able to reproduce the characteristic shape of these tumors which is in itself a very satisfactory result. Furthermore, from this model we have derived a simpler non-spatial model able to reproduce the 4 different types of response to radiotherapy observed by clinicians on the more than 70 patients they have selected for this study.
- Theoretical biology of the metastatic process
  We proposed a theoretical study of systemic inhibition of angiogenesis (SIA) in a population of tumors by deriving a model from biophysical considerations and simulating a novel mathematical model able to describe the development of a population of tumors in mutual inhibitory interactions at the organism scale. We showed that the model could explain experimental data on metastatic development and tested the hypothesis of global dormancy (cancer without disease) resulting from the net inhibitory action of stimulatory and inhibitory signaling interactions among the lesions comprising the total tumor burden. We found SIA alone is not sufficient for global dormancy but could suppress the growth of the total metastatic burden. See [41]. The resulting model is a nonlinear partial differential transport equation with nonlocal boundary condition that describes organism-scale population dynamics under the influence of three processes: birth (dissemination of secondary tumors), growth and inhibition (through angiogenesis). The asymptotic behavior of the model was numerically investigated in a second publication [40] and revealed interesting dynamics ranging

from convergence to a steady state to bounded non-periodic or periodic behaviors, possibly with complex repeated patterns.

In link with the previous study and in order to base the modeling on relevant biological data studying the basic phenomenon of growth interactions among tumors, we first performed a rational, quantitative and discriminant analysis of the descriptive and predictive properties of classical ODE-based models for tumor volume kinetics, which has been summarized in a publication that is currently under revision for PloS Computational Biology [42].

A collaboration with John Ebos from the Roswell Park Cancer Institute in Buffalo (NY, USA) has been initiated that deals with the objectives to quantify metastatic aggressiveness of several cancer cell linesand to rationally define a neo-adjuvant (i.e., prior to resection of the primary lesion) efficacy score of several anti-cancer chemical agents. The PhD of Etienne Baratchart has been initiated, in close collaboration with the "Angiogenesis and cancer microenvironment laboratory" directed by the Pr Andreas Bikfalvi, about the initiation, development and role of the pre-metastatic and metastatic niche.

6.2. Newtonian fluid flows simulations and their analysis

- Simulations of water distribution systems :Water losses may constitute a large amount of the distributed total water volume throughout water distribution systems. Here, a new model method is proposed that intends to minimize the total water volume distributed through leakage reduction. Our group has worked on the derivation of advection-reaction-diffusion type equations with an explicit relationship between the local pressure and the leakage rate. An original splitting technique to solve this type of hydraulic problem was then achieved. This technique allows pressure-dependent leakage to be taken into account, whereas in most models leakage is assumed to be uniform along a pipe. Finally, a constrained optimization problem was formulated for leakage reduction in WDS. The control variable had the mean of a local head loss and is considered in the Boundary Conditions to avoid dealing with discontinuities in the governing equations. The objective function to minimize was a regularization of the total water volume distributed. Specific operational constraints were added to ensure enough pressure at consumption points. The direct solution for this minimization problem was sought with a Gradient type method. The leakage reduction was proven to be significant in a case study. The percentage of leakage reduced from 24% to 10% in the linear relationship between pressure and leakage flow rate. With other leakage exponents, the same rate of reduction was achieved . The method was applied on a real network in the South-West of France. Controlling the pressure at two different strategic points permits a significant amount of the total distributed water to be saved (5%). This work was performed in collaboration with Cemagref Bordeaux . Future work will consist of applying a sensibility analysis of control location points to optimize the method.
- Incompressible flows : modeling and simulation of moving and deformable bodies. The incompressible Navier-Stokes equations are discretized in space onto a fixed cartesian mesh. The deformable bodies are taken into using a first order penalization method and/or second order immersed boundary method. The interface between the solid and the fluid is tracked using a level-set description so that it is possible to simulate several bodies freely evolving in the fluid. A turbulence model based on Samgorinsky model has been added to the numerical code. The numerical code written in the C langage is massively parallel. The large linear systems (over than 100 millions of dofs) are solved using the Petsc Library. As an illustration of the methods, fish-like locomotion is analyzed in terms of propulsion efficiency. Underwater maneuvering and school swimming are also explored. We were able to simulate the three-dimensional flow about a swimmer for realistic physical configurations. Another application is the turbulent 3D flow around complex wind turbine (see http://www.math.u-bordeaux1.fr/~mbergman and http://www.math.u-bordeaux1.fr/MAB/mc2/analysis.html for simulation movies). Wake flows generated by boat propellers are also modeled and simulated.
  We recently take in account a simplified elasticity model of the swimmer (elastic caudal tail of a fish). Some elastic parameters allows to increase the swimming efficiency around 20%-30%.

Recent developments on multiphase flows have been performed. We are able to simulate water/air interactions with interface regularization. The interface with a boat is also taken into account. See http://www.math.u-bordeaux1.fr/~mbergman for simulations.
We are also able to compute the strong (implicit) fluid structure interactions between the fluid and an elastic medium. For instance we have simulated a fish with an elastic tail and highlighted the fact that a given flexibility of tail allows to increase significantly the swimming efficiency.

- Turbulence flow on an hemisphere : Participants: Charles-Henri Bruneau, Patrick Fischer (MCF Bordeaux 1), Yong Liang Xiang (PostDoc)
  ANR Cyclobulle lead by Hamid Kellay Soap hemi-bubble film experiments have shown some links between the formation of vortices when the hemi-bubble is heated at the equator and the formation of tornados in the earth atmosphere. Two-dimensional simulations using a stereographic map are used to compare to these experimental results and confirm the results when Coriolis force and heat source terms are added.
- Compressible flows: Immersed boundary methods. We are concerned with immersed boundary methods, i.e., integration schemes where the grid does not fit the geometry, and among this class of methods, more specifically with cartesian grid methods, where the forcing accounting for the presence of boundaries is performed at the discrete level. We have developed a simple globally second order scheme inspired by ghost cell approaches to solve compressible flows, inviscid as well as viscous. In the fluid domain, away from the boundary, we use a classical finite-volume method based on an approximate Riemann solver for the convective fluxes and a centered scheme for the diffusive term. At the cells located on the boundary, we solve an ad hoc Riemann problem taking into account the relevant boundary condition for the convective fluxes by an appropriate definition of the contact discontinuity speed. This method can easily be implemented in existing codes and is suitable for massive parallelization. It has been validated in two dimensions for Euler and Navier-Stokes equations, and in three dimensions for Euler equations. The order of convergence is two in L^2 norm for all variables, and between one and two in L^∞ depending on the variables. The 3D code has been parallelized with MPI. The case of a moving solid has been tested (flapping wing) and gives results for the drag and the lift in agreement with the references in the literature.
  The Oldroyd B constitutive model is used to study the role of the viscoelasticity of dilute polymer solutions in two-dimensional flows past a bluff body using numerical simulations. This investigation is motivated by the numerous experimental results obtained in quasi two dimensional systems such as soap film channels. The numerical modeling is novel for this case and therefore a comprehensive comparison is carried out to validate the present penalization method and artificial boundary conditions. In particular we focus on flow past a circular object for various values of the Reynolds number, Weissenberg number, and polymer viscosity ratio. Drag enhancement and drag reduction regimes are discussed in detail along with their flow features such as the pattern of vortex shedding, the variation of lift as well as changes in pressure, elongational rates, and polymer stress profiles. A comprehensive study of the flow behavior and energy balance are carefully carried out for high Reynolds numbers. Flow instabilities in both numerical and experimental results are discussed for high Weissenberg numbers .
- Elliptic problems: We have developed a new cartesian method to solve elliptic problems with immersed interfaces. These problems appear in numerous applications, among them: heat transfer, electrostatics, fluid dynamics, but also tumour growth modelling, or modelling of electric potential in biological cells This method is second order accurate in the whole domain, notably near the interface. The originality of the method lies on the use of additionnal unknows located on interface points, on which are expressed flux equalities. Special care is dedicated to the discretization near the interface, in order to recover a stable second order accuracy. Actually, a naive discretization could lead to a first order scheme, notably if enough accuracy in the discretization of flux transmission condtions is not provided. Interfaces are represented with a distance level-set function discretized on the grid points. The method has been validated on several test-cases with complex interfaces in 2D. A parallel version has been developed using the PETSC library.

- Simulations of fluid-solid interactions : The interaction of an elastic structure and an fluid occurs in many phenomena in physics. To avoid the difficulty of coupling lagrangian elasticity with an eulerian fluid we consider a whole eulerian formulation. The elasticity of the structure is computed with retrograde caracteristics which satisfy a vectorial transport equation. We derive the associated fluid-structure models for incompressible and compressible media. The equations are discretized on a cartesian mesh with finite differences and finite volumes schemes. The applications concern the bio-locomotions and the study of air-elastic interaction.
- Vortex methods : The aim of this work is to couple vortex methods with the penalization methods in order to take advantage from both of them. This immersed boundary approach maintains the efficiency of vortex methods for high Reynolds numbers focusing the computational task on the rotational zones and avoids their lack on the no-slip boundary conditions replacing the vortex sheet method by the penalization of obstacles. This method that is very appropriate for bluff-body flows is validated for the flow around a circular cylinder on a wide range of Reynolds numbers. Its validation is now extended to moving obstacles (axial turbine blades) and three-dimensional bluff-bodies (flow around a sphere). See [72]. Moreover, using the global properties of the penalization method, this technique permits to include porous media simultaneously in the flow computation. We aim to adapt the porous media flows to our new method and to apply it in order to implement passive control techniques using porous layers around bluff-bodies.
- Domain decomposition : Domain decomposition methods are a way to parallelize the computation of numerical solutions to PDE. To be efficient, domain decompositions methods should converge independently on the number of subdomains. The classical convergence result for the additive Schwarz preconditioner with coarse grid is based on a stable decomposition. The result holds for discrete versions of the Schwarz preconditioner, and states that the preconditioned operator has a uniformly bounded condition number that depends only on the number of colors of the domain decomposition, and the ratio between the average diameter of the subdomains and the overlap width. Constants are usually non explicit and are only asserted to depend on the "shape regularity" of the domain decomposition.
  two years ago, we showed the result holds the additive Schwarz preconditioner can also be defined at the continuous level and provided completely explicits estimates. Last year, we established that a similar result also holds for non shape regular domain decompositions where the diameter of the smallest subdomain is significantly smaller than the diameter of the largest subdomain. The constants are also given explicitely and are independent of the ratio between the diameter of the largest sudomain and the diameter of the smallest subdomain.
  This year, we have studied explored new coarse spaces algorithms for domain decomposition methods. Coarse spaces are necessary to get a scalable algorithm whose convergence speed does not deteriorate when the number of subdomains increases. For domains decomposition methods with discontinuous iterates, we showed that continuous coarse spaces can never be an optimal choice. As an alternative, we introduced both the use of discontinuous coarse spaces(DCS) and a new coarse space algorithm using these discontinuous coarse spaces.

6.3. Flow control and shape optimization

- Flow control : Participants: Charles-Henri Bruneau, Iraj Mortazavi, Emmanuel Creusé (Lille), Patrick Gilliéron (Paris).

  An efficient active control of the two- and three-dimensions flow around the 25 degrees rear window Ahmed body has been performed. A careful theoretical and numerical study of the trajectories of the vortices allows to adapt the control in order to improve its efficiency and get a better drag reduction.

MOKAPLAN Exploratory Action

6. New Results

6.1. Monge-Ampère solver for the Mass Transportation problem and extensions

- **Benamou, Froese (Univ. of Texas at Austin) -** We design a scheme for Aleksandrov solution of Optimal Mass Transportation between atomic measure and continuous densities. The idea is to couple the notion of viscosity solution with an adapted sub gradient discretization at dirac points where the notion of Aleksandrov solution is relevant. This would offer a "PDE" alternative to the classical gradient methods based on costly computational geometry tools [61].
- **Benamou, Collino, Mirebeau (Univ. Paris IX,CNRS) -** A new variational formulation of the determinant of a semi-definite positive matrix has been proposed based on the ideas developed in [60]. This leads to a monotone discretisation of the Monge-Ampère operator. A Newton method preserving convexity is currently being tested. The new scheme is more accurate than the wide stencil, currently the state of the art of monotone scheme for the Monge-Ampère equation.
- **Benamou, Froese (Univ. of Texas at Austin), Oberman (Univ. Mc Gill) -** When the Optimal Mass Transportation data is not balanced, i.e. the densities do not have equal mass. A natural extension of the optimal transport has been proposed by McCann and Caffareli [30] and revisited by Figalli [41]. It is formulated as an obstacle problem which automatically select the portion of mass corresponding to Optimal Mass Transportation. The numerical resolution of this problem is open and we believe ideas linked the state constraint reformulation contained in paper [6] may be applied to obtain a tractable reformulation.

6.2. Variational problems under divergence constraint - Alg2

- **Benamou, Bonne, Carlier -** Dynamic problems: we have extended the Augmented Lagrangian method used for the CFD formulation of the Optimal Mass Transportation to Mean Field Games that is for the optimal control of the continuity equation. A freefem Code has been implemented.
- **Benamou, Carlier -** Static problems with a divergence constraint. We have also extended the Augmented Lagrangian method to static problem where a space divergence constraint appears. This includes the delicate case of the original Monge Optimal Mass Transportation cost (cost=distance) and also Wardrop equilibria in congested transport and related degenerate elliptic equations, like the p-Laplacian operator. A freefem Code has been implemented.

6.3. Multi-marginal problems

- **[Carlier, Oberman (Univ. Mc Gill), Oudet (Univ. of Grenoble) -** New numerical methods for the Wasserstein barycenter and related multi-marginals problems were investigated [49]. A first method uses linear programming, in an implementation that was more efficient than expected. A second method takes advantage of the quadratic structure and leads to an efficient algorithm that can be used in texture synthesis problems arising in image processing.
- **Benamou, Carlier, Nenna** Extension of the CFD formulation and the ALG2 algorithm to the multi marginal problem with quadratic cost (Barycenter).

6.4. JKO gradient flow numerics

Figure 2. Monge transport flow between sinks and sources.

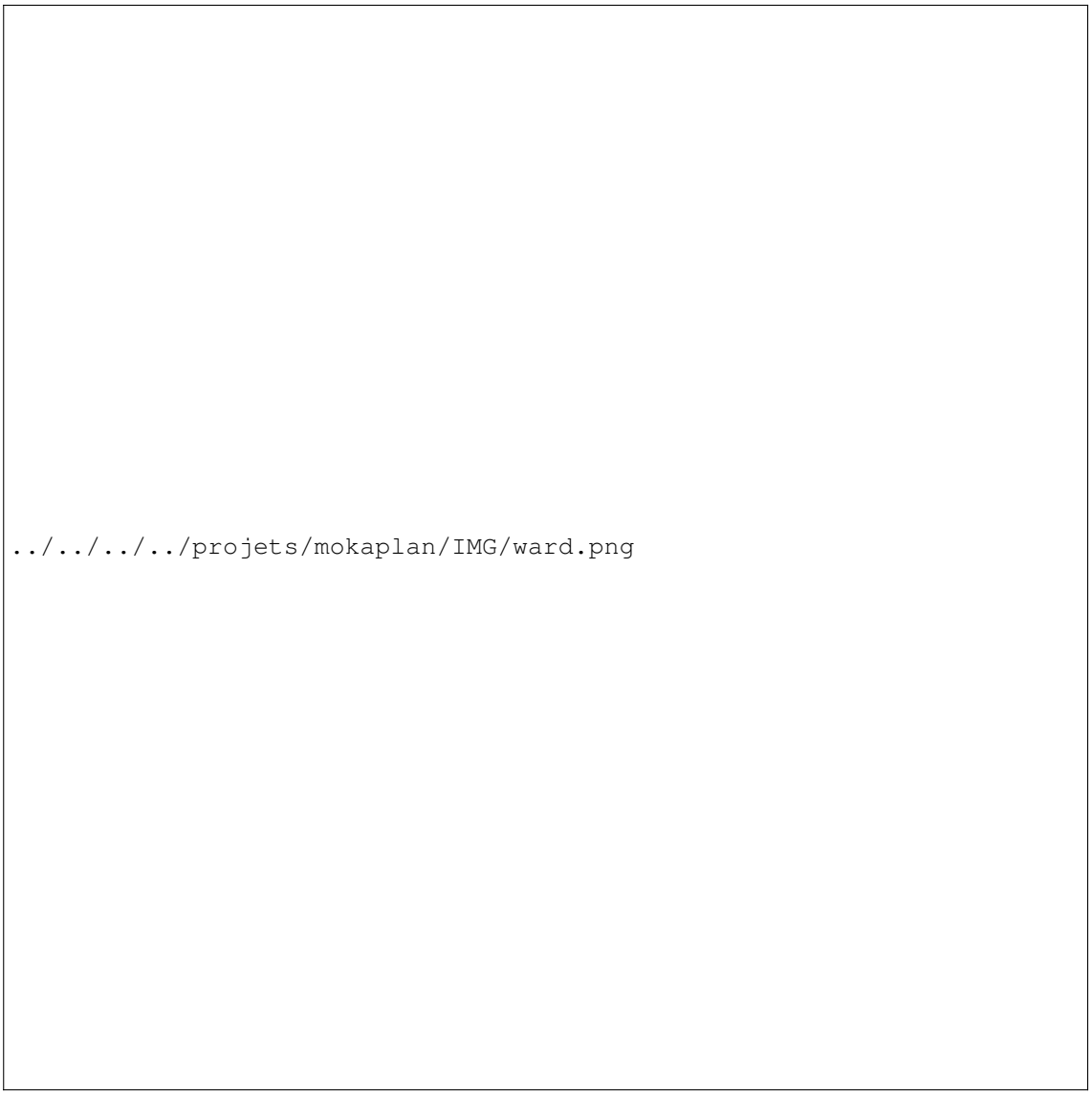


Figure 3. Congested transport flows between sink and source.

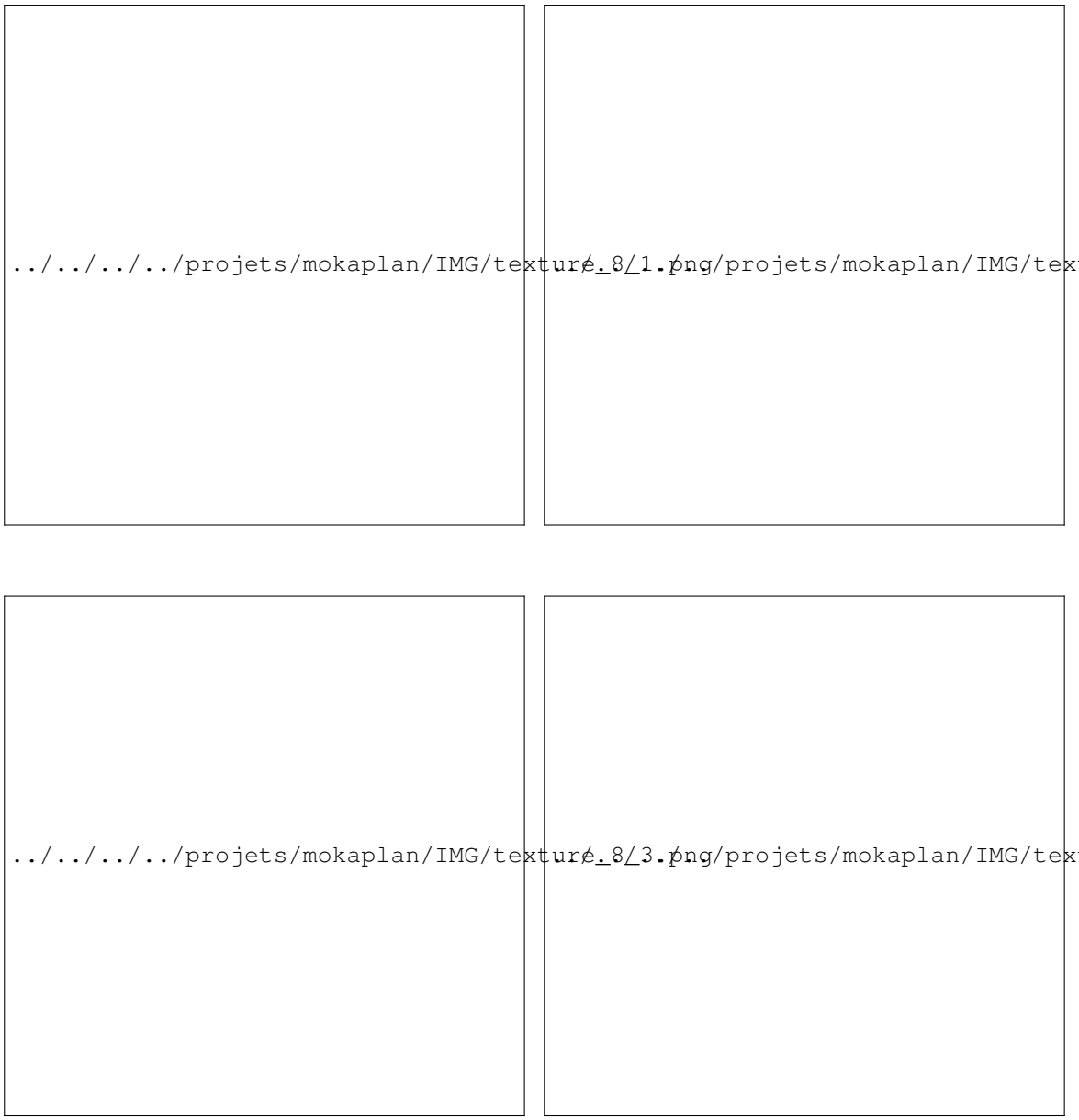


Figure 4. Texture mixing with Wasserstein barycenters, from top to bottom three densities and their barycenter.

- **Benamou, Carlier, Merigot (Univ. of Grenoble, CNRS) , Oudet (Univ. of Grenoble)**q

  A large class of non-linear continuity equations with confinement and/or possibly non local interaction potential can be considered as semi discrete gradient flows with respect to the Euclidean Wassertein distance. The numerical resolution of such problem in dimension 2 and higher is open. Our approach is based on two remarks : the reformulation of the optimization problem in terms of Brenier potential seems to behave better. This introduces a Monge-Ampère operator in the cost functional which needs a monotone discretization in order to preserve the convexity at the discrete level. The first numerical results are very encouraging.

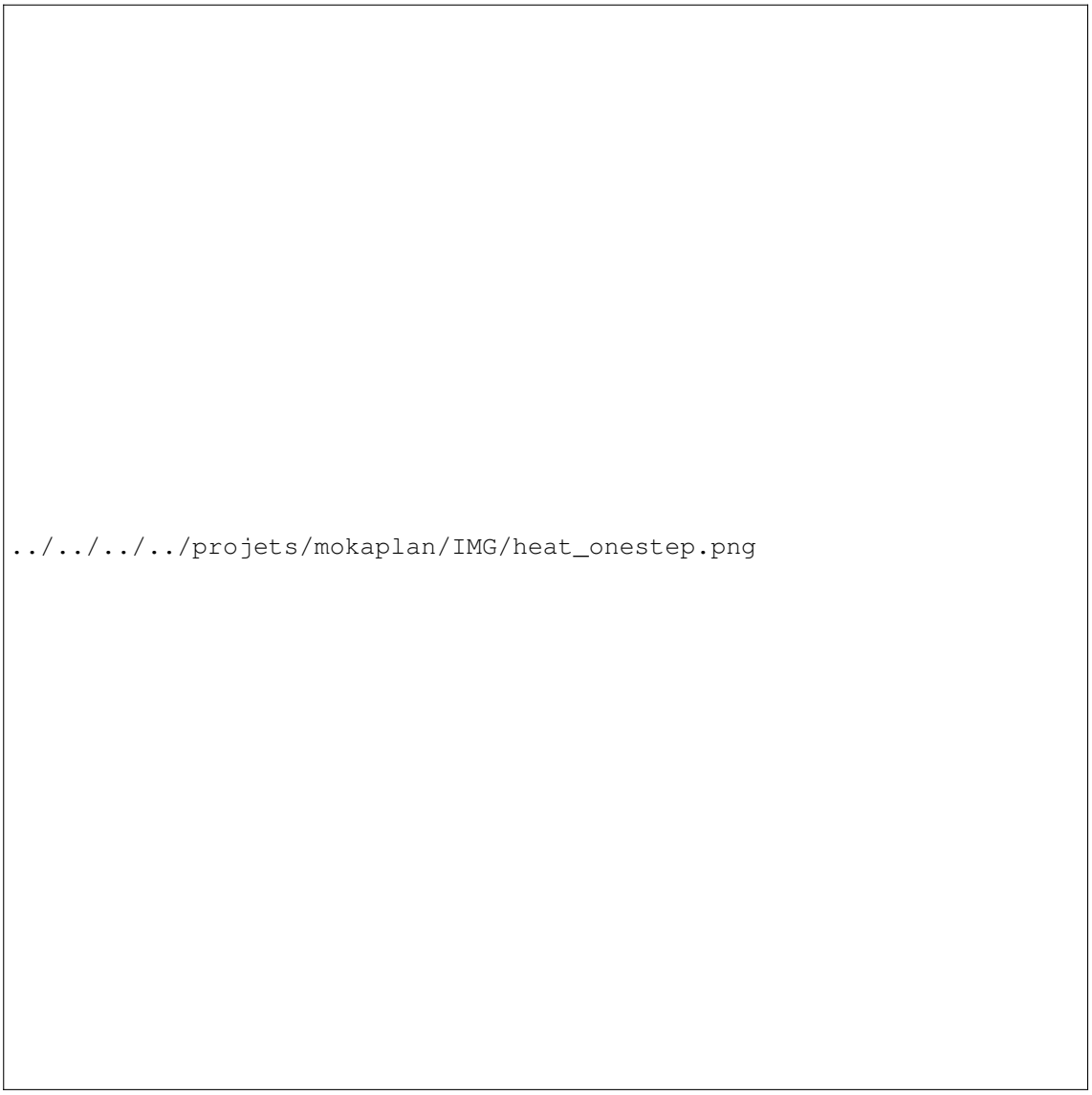


Figure 5. One step of Wasserstein JKO gradient flow for the classical entropy (our numerical method) compared to traditional Finite Difference of the heat equation. Left the initial heat profile, right the heat profile after one time step for both methods.

- **Benamou, Carlier, Agueh (Univ. of Victoria)** Splitting methods for kinetic equations, we try to use one JKO step to deal with the non-linear velocity advection part of kinetic equations [31]. This seems to be relevant to granular media equation [16], and also may offer a completely new method for Liouville equations arising from Geometrical Optics [19].

NACHOS Project-Team

6. New Results

6.1. Discontinuous Galerkin methods for Maxwell's equations

6.1.1. DGTD-$\mathbb{P}_p$ method based on hierarchical polynomial interpolation

Participants: Loula Fezoui, Stéphane Lanteri.

The DGTD (Discontinuous Galerkin Time Domain) method originally proposed by the team for the solution of the time domain Maxwell's equations [16] relies on an arbitrary high order polynomial interpolation of the component of the electromagnetic field, and its computer implementation makes use of nodal (Lagrange) basis expansions on simplicial elements. The resulting method is often denoted by DGTD-$\mathbb{P}_p$ where p refers to the interpolation degree that can be defined locally i.e. at the element level. In view of the design of a hp-adaptive DGTD method, i.e. a solution strategy allowing an automatic adaptation of the interpolation degree p and the discretization step h, we now investigate alternative polynomial interpolation and in particular those which lead to hierarchical or/and orthogonal basis expansions. Such basis expansions on simplicial elements have been extensively studied in the context of continuous finite element formulations (e.g. [59]) and have thus been designed with global conformity requirements (i.e. H_1, $H(\mathrm{rot})$ or (div)) whose role in the context of a discontinuous Galerkin formulation has to be clarified. This represents one of the objectives of this study. This year, we have started the development of a new software platform in Fortran 95 implementing DGTD-$\mathbb{P}_p$ able to deal with different polynomial basis expansions on a tetrahedral element, for the solution of the 3D time domain Maxwell equations.

6.1.2. DGTD-$\mathbb{P}_p\mathbb{Q}_k$ method on multi-element meshes

Participants: Clément Durochat, Stéphane Lanteri, Raphael Léger, Claire Scheid, Mark Loriot [Distene, Pôle Teratec, Bruyères-le-Chatel].

In this work, we study a multi-element DGTD method formulated on a hybrid mesh which combines a structured (orthogonal) discretization of the regular zones of the computational domain with an unstructured discretization of the irregularly shaped objects. The general objective is to enhance the flexibility and the efficiency of DGTD methods for large-scale time domain electromagnetic wave propagation problems with regards to the discretization process of complex propagation scenes. With this objective in mind, we have designed and analyzed a DGTD-$\mathbb{P}_p\mathbb{Q}_k$ method formulated on non-conforming hybrid quadrangular/triangular meshes (2D case) or non-conforming hexahedral/tetrahedral meshes (3D case) for the solution of the time domain Maxwell's equations [23]-[22].

6.1.3. DGTD-$\mathbb{P}_p$ method for Debye media and applications to biolectromagnetics

Participants: Claire Scheid, Maciej Klemm [Communication Systems & Networks Laboratory, Centre for Communications Research, University of Bristol, UK], Stéphane Lanteri.

This work is undertaken in the context of a collaboration with the Communication Systems & Networks Laboratory, Centre for Communications Research, University of Bristol (UK). This laboratory is studying imaging modalities based on microwaves with applications to dynamic imaging of the brain activity (Dynamic Microwave Imaging) on one hand, and to cancerology (imaging of breast tumors) on the other hand. The design of imaging systems for these applications is extensively based on computer simulation, in particular to assess the performances of the antenna arrays which are at the heart of these systems. In practice, one has to model the propagation of electromagnetic waves emitted from complex sources and which propagate and interact with biological tissues. In relation with these issues, we study the extension of the DGTD-$\mathbb{P}_p$ method originally proposed in [16] to the numerical treatment of electromagnetic wave propagation in dispersive media. We consider an approach based on an auxiliary differential equation modeling the time evolution of the electric polarization for a dispersive medium of Debye type (other dispersive media will be considered subsequently). The stability and a priori convergence analysis of the resulting DGTD-$\mathbb{P}_p$ method has been studied [25], and its application to the simulation of the propagation in realistic geometrical models of head tissues is underway in the context of our participation to the DEEP-ER FP7 project.

Figure 4. Scattering of a plane wave by a disk. Conforming triangular mesh (top left) and non-conforming quadrangular/triangular mesh (top right). Contour lines of electrical field component E_z from a simulation with a DGTD-$\mathbb{P}_2\mathbb{Q}_4$ method (bottom).

6.1.4. DGTD-$\mathbb{P}_p$ method for nanophotonics

Participants: Claire Scheid, Maciej Klemm [Communication Systems & Networks Laboratory, Centre for Communications Research, University of Bristol, UK], Stéphane Lanteri, Raphael Léger, Jonathan Viquerat.

Modelling and numerical simulation aspects are crucial for a better understanding of nanophotonics. Media that one encounters are complex and the geometries quite involved, so that while a FDTD method failed to be accurate enough, a non conforming discretisation method seems to be well adapted. In this direction, since the end of 2012, we are actively studying the numerical modeling of electromagnetic wave interaction with nanoscale metallic structures. In this context, one has to take into account the dispersive characteristics of metals in the frequency range of interest to nanophotonics. As a first step in this direction, we have considered an auxiliary differential equation approach for the numerical treatment of a Drude, Drude-Lorentz and a generalized dispersion models in the framework of a DGTD-$\mathbb{P}_p$ method [20]-[36]. We performed the corresponding numerical analysis as well as numerical validation tests cases. Some methodological improvements, such as curvilinear elements and higher order time discretization schemes are also underway.

6.1.5. Frequency domain hybridized DGFD-$\mathbb{P}_p$ methods

Participants: Stéphane Lanteri, Liang Li [Faculty Member, School of Mathematical Sciences, Institute of Computational Science, University of Electronic Science and Technology of China Chengdu, China], Ronan Perrussel [Laplace Laboratory, INP/ENSEEIHT/UPS, Toulouse].

For certain types of problems, a time harmonic evolution can be assumed leading to the formulation of the frequency domain Maxwell equations, and solving these equations may be more efficient than considering the time domain variant. We are studying a high order Discontinuous Galerkin Frequency Domain (DGFD-$\mathbb{P}_p$) method formulated on unstructured meshes for solving the 2D and 3D time harmonic Maxwell equations. However, one major drawback of DG methods is their intrinsic cost due to the very large number of globally coupled degrees of freedom as compared to classical high order conforming finite element methods. Different attempts have been made in the recent past to improve this situation and one promising strategy has been recently proposed by Cockburn *et al.* [48] in the form of so-called hybridizable DG formulations. The distinctive feature of these methods is that the only globally coupled degrees of freedom are those of an approximation of the solution defined only on the boundaries of the elements. This work is concerned with the study of such Hybridizable Discontinuous Galerkin (HDG) methods for the solution of the system of Maxwell equations in the time domain when the time integration relies on an implicit scheme, or in the frequency domain. We have been one of the first groups to study HDGFD-$\mathbb{P}_p$ methods based on nodal interpolation methods for the solution of the 2D and 3D frequency domain Maxwell equations [26]-[27].

6.1.6. Exact transparent condition in a DGFD-$\mathbb{P}_p$ method

Participants: Mohamed El Bouajaji, Nabil Gmati [ENIT-LAMSIN, Tunisia], Stéphane Lanteri, Jamil Salhi [ENIT-LAMSIN, Tunisia].

In the numerical treatment of propagation problems theoretically posed in unbounded domains, an artificial boundary is introduced on which an absorbing condition is imposed. For the frequency domain Maxwell equations, one generally use the Silver-Müller condition which is a first order approximation of the exact radiation condition. Then, the accuracy of the numerical treatment greatly depends on the position of the artificial boundary with regards to the scattering object. In this work, we have conducted a preliminary study aiming at improving this situation by using an exact transparent condition in place of the Silver-Müller condition. Promising results have been obtained in the 2D case [30].

6.2. Discontinuous Galerkin methods for the elastodynamic equations

6.2.1. DGTD-$\mathbb{P}_p$ method for viscoelastic media

Participants: Nathalie Glinsky, Stéphane Lanteri, Fabien Peyrusse.

We continue developing high order non-dissipative discontinuous Galerkin methods on simplicial meshes for the numerical solution of the first order hyperbolic linear system of elastodynamic equations. These methods share some ingredients of the DGTD-$\mathbb{P}_p$ methods developed by the team for the time domain Maxwell equations among which, the use of nodal polynomial (Lagrange type) basis functions, a second order leap-frog time integration scheme and a centered scheme for the evaluation of the numerical flux at the interface between neighboring elements. The resulting DGTD-$\mathbb{P}_p$ methods have been validated and evaluated in detail in the context of propagation problems in both homogeneous and heterogeneous media including problems for which analytical solutions can be computed. Particular attention was given to the study of the mathematical properties of these schemes such as stability, convergence and numerical dispersion.

A recent novel contribution is the extension of the DGTD method to include viscoelastic attenuation. For this, the velocity-stress first-order hyperbolic system is completed by additional equations for the anelastic functions including the strain history of the material. These additional equations result from the rheological model of the generalized Maxwell body and permit the incorporation of realistic attenuation properties of viscoelastic material accounting for the behaviour of elastic solids and viscous fluids. In practice, we need solving 3L additional equations in 2D (and 6L in 3D), where L is the number of relaxation mechanisms of the generalized Maxwell body. This method has been implemented in 2D and validated by comparison to results obtained by a finite-difference method, in particular for wave propagation in a realistic basin of the area of Nice (south of France)

6.2.2. DGTD-$\mathbb{P}_p$ method for the assessment of topographic effects

Participants: Etienne Bertrand [CETE Méditerranée], Nathalie Glinsky.

This study addresses the numerical assessment of site effects especially topographic effects. The study of measurements and experimental records proved that seismic waves can be amplified at some particular locations of a topography. Numerical simulations are exploited here to understand further and explain this phenomenon. The DGTD-$\mathbb{P}_p$ method has been applied to a realistic topography of Rognes area (where the Provence earthquake occured in 1909) to model the observed amplification and the associated frequency. Moreover, the results obtained on several homogeneous and heterogeneous configurations prove the influence of the medium in-depth geometry on the amplifications measures at the surface .

6.2.3. DGTD-$\mathbb{P}_p$ method for arbitrary heterogeneous media

Participants: Nathalie Glinsky, Diego Mercerat [CETE Méditerranée].

We have recently devised an extension of the DGTD method for elastic wave propagation in arbitrary heterogeneous media. In realistic geological media (sedimentary basins for example), one has to include strong variations in the material properties. Then, the classical hypothesis that these properties are constant within each element of the mesh can be a severe limitation of the method, since we need to discretize the medium with very fine meshes resulting in very small time steps. For these reasons, we propose an improvement of the DGTD method allowing non-constant material properties within the mesh elements. A change of variables on the stress components allows writing the elastodynamic system in a pseudo-conservative form. Then, the introduction of non-constant material properties inside an element is simply treated by the calculation, via convenient quadrature formulae, of a modified local mass matrix depending on these properties. This new extension has been validated for a smoothly varying medium or a strong jump between two media, which can be accurately approximated by the method, independently of the mesh .

6.2.4. DGFD-$\mathbb{P}_p$ method for frequency domain elastodynamics

Participants: Hélène Barucq [MAGIQUE3D project-team, Inria Bordeaux - Sud-Ouest], Marie Bonnasse, Julien Diaz [MAGIQUE3D project-team, Inria Bordeaux - Sud-Ouest], Stéphane Lanteri.

We have started this year a research direction aiming at the development of high order discontinuous Galerkin methods on unstructured meshes for the simulation of frequency domain elastodynamic and viscelastic wave propagation. This study is part of the Depth Imaging Partnership (DIP) between Inria and TOTAL. The PhD thesis of Marie Bonnasse is at the heart of this study which is funded by TOTAL.

6.3. Multiscale finite element methods for time-domain wave models

Participants: Marie-Helene Lallemand Tenkes, Stéphane Lanteri, Claire Scheid, Frédéric Valentin [LNCC, Petrópolis, Brazil].

Mathematical (partial differential equation) models embedding multiscale features occur in a wide range of natural situations and industrial applications involving wave propagation. This is for instance the case of electromagnetic or seismic wave propagation in heterogenous media. Although the related applications take place at the macro-scale, it is well known that the parameters describing the macro-scale processes are eventually determined by the solution behavior at the micro-sacle. As a result, each stage of the modeling of the underlying problem is driven by distinct sets of PDEs with highly heterogeneous coefficients and embedded high-contrast interfaces. Because of the huge difference in physical scales in heterogenous media it is not computationally feasible to fully resolve the micro-scale features directly. Macroscopic models or upscaling techniques have therefore to be developed that are able to accurately capture the macroscopic behavior while significantly reducing the computational cost. In this context, researchers at LNCC have recently proposed a new family of finite element methods [51]- [50], called Multiscale Hybrid-Mixed methods (MHM), which is particularly adapted to be used in high-contrast or heterogeneous coefficients problems. Particularly, they constructed a family of novel finite element methods sharing the following properties: (i) stable and high-order convergent; (ii) accurate on coarse meshes; (iii) naturally adapted to high-performance parallel computing; (iv) induce a face-based a posteriori error estimator (to drive mesh adaptativity); (v) locally conservative. We have started this year a new reserach direction aiming at the design of similar MHM methods for solving PDE models of time-domain electromagnetic and seismic wave propagation.

6.4. Time integration strategies and resolution algorithms

6.4.1. Hybrid explicit-implicit DGTD-$\mathbb{P}_p$ method

Participants: Stéphane Descombes, Stéphane Lanteri, Ludovic Moya.

Existing numerical methods for the solution of the time domain Maxwell equations often rely on explicit time integration schemes and are therefore constrained by a stability condition that can be very restrictive on highly refined meshes. An implicit time integration scheme is a natural way to obtain a time domain method which is unconditionally stable. Starting from the explicit, non-dissipative, DGTD-$\mathbb{P}_p$ method introduced in [16], we have proposed the use of Crank-Nicolson scheme in place of the explicit leap-frog scheme adopted in this method [5]. As a result, we obtain an unconditionally stable, non-dissipative, implicit DGTD-$\mathbb{P}_p$ method, but at the expense of the inversion of a global linear system at each time step, thus obliterating one of the attractive features of discontinuous Galerkin formulations. A more viable approach for 3D simulations consists in applying an implicit time integration scheme locally i.e in the refined regions of the mesh, while preserving an explicit time scheme in the complementary part, resulting in an hybrid explicit-implicit (or locally implicit) time integration strategy. In [7], we conducted a preliminary numerical study of a hyrbid explicit-implicit DGTD-$\mathbb{P}_p$ method, combining a leap-frog scheme and a Crank-Nicolson scheme, and obtained promising results. More recently, we further investigated two such strategies, both theoretically (especially, convergence in the ODE and PDE senses) [17] and numerically in the 2D case [28]. A last topic is to propose higher order time integration techniques based on the second-order locally implicit method to fully exploit the attractive features of this approach combined with a DG discretisation which allows to easily increase the spatial convergence order. Promising results in 2D reaching high order in time, between $3, 5$ and 4, have been obtained in [29] by applying Richardson extrapolation and composition methods.

6.4.2. Optimized Schwarz algorithms for the frequency domain Maxwell equations

Participants: Victorita Dolean, Martin Gander [Mathematics Section, University of Geneva], Stéphane Lanteri, Ronan Perrussel [Laplace Laboratory, INP/ENSEEIHT/UPS, Toulouse].

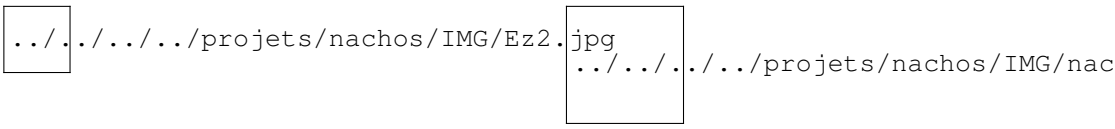
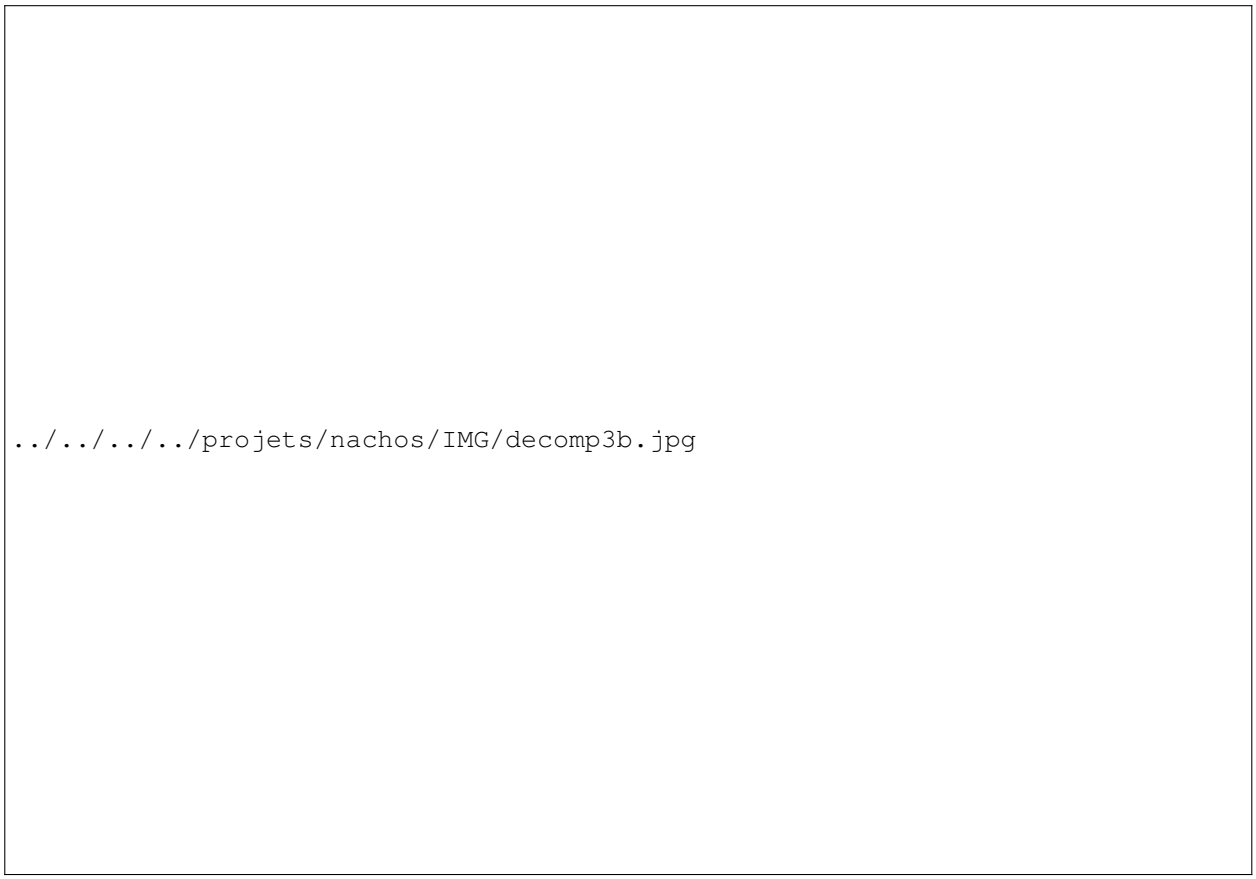


Figure 5. Scattering of a plane wave by an airfoil profile. Contour lines of electrical field component E_z (left) and locally refined triangular mesh with partitioning in explicit/implicit zones (right).

Even if they have been introduced for the first time two centuries ago, over the last two decades, classical Schwarz methods have regained a lot of popularity with the developement of parallel computers. First developed for the elliptic problems, they have been recently extended to systems of hyperbolic partial differential equations, and it was observed that the classical Schwartz method can be convergent even without overlap in certain cases. This is in strong contrast to the behavior of classical Schwarz methods applied to elliptic problems, for which overlap is essential for convergence. Over the last decade, optimized versions of Schwarz methods have been developed for elliptic partial differential equations. These methods use more effective transmission conditions between subdomains, and are also convergent without overlap for elliptic problems. The extension of such methods to systems of equations and more precisely to Maxwell's system (time harmonic and time discretized equations) has been studied in [9]. The optimized interface conditions proposed in [9] were devised for the case of non-conducting propagation media. We have recently studied the formulation of such conditions for conducting media [4]. Besides, we have also proposed an appropriate discretization strategy of these optimized Schwarz algorithms in the context of a high order DGFD-$\mathbb{P}_p$ method formulated on unstructured triangular meshes for the solution of the 2D frequency domain Maxwell equations [42].



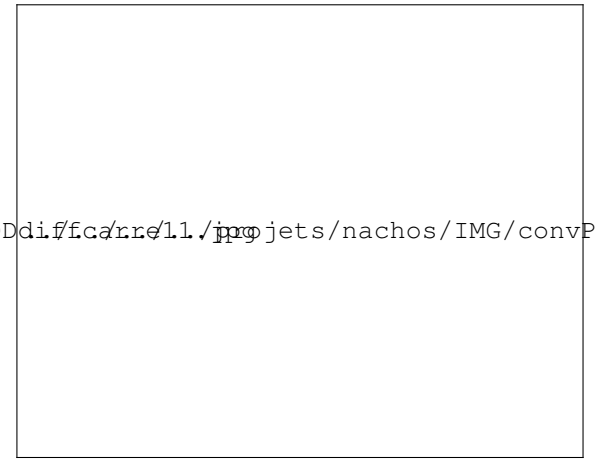


Figure 6. Propagation of a plane wave in a multilayered heterogeneous medium. Problem setting and two-subdomain decompositin (top). Contour lines of the real part of the E_z component of the electrical field (bottom left) and asymptotic convergence of the optimized Schwarz algorithms (bottom right).

NANO-D Team

5. New Results

5.1. Adaptively Restrained Particle Simulations for Isobaric-Isothermal Ensemble

Participants: Zofia Trstanova, Stephane Redon.

We continued working on the Adaptively Restrained Particles Simulations (ARPS) approach that was proposed by Svetlana Artemova and Stephane Redon [11] and that was designed to speed up the particles simulations by switching on and off the degrees of freedom based on the kinetic energy of the particle.

It has been shown, for the NVE and the NVT ensemble, that this method has many advantages [11]. We want to extend ARPS for the isobaric-isothermal ensemble (NPT) since this ensemble is very often used in particle simulations, because many chemical reactions happen under constant pressure. An adaptive method for this ensemble with advantages of ARPS might be very useful in many scientific domains (physics, biology, chemistry).

We combined the ARPS method with an existing method that describes the NPT ensemble. We already obtained very promising analytical and numerical results that support the main characteristically advantages of ARPS shown by Svetlana Artemova and Stephane Redon. For instance, Figure 4 shows preservation of the radial distribution function.

5.2. Interactive large-scale deformations of molecular structures

Participants: Jelmer Wolterink, Himani Singhal, Marc Piuzzi, Stephane Redon.

We have developed new interaction methods for large-scale deformation of molecular structures. These new methods allow a user to attach control points to molecules, and use these control points to easily deform the structures while preserving their realism (e.g. local interactions, etc.). The new methods may be applied to any type of molecule (e.g. proteins, carbon nanotubes, etc.), and may be used in combination with interactive simulation.

5.3. Towards parallel adaptive molecular simulations

Participants: Krishna Kant Singh, Benjamin Bouvier, Jean-Francois Mehaut, Stephane Redon.

The adaptive algorithms that we are developing have two main components. The first component determines when and how degrees of freedom can be deactivated and reactivated during a simulation. The second component takes advantage of the frozen degrees of freedom to accelerate the calculation of the potential energy and interatomic forces. Indeed, the potential energy and forces can often be expressed as a (potentially complex) sum of terms which only depend on relative atomic positions. When the relative positions do not change, it is not necessary to update the corresponding terms, which reduces the computation time. We have shown that it is possible to significantly speed up simulations using this approach, while being able to recover static equilibrium statistics [11].

We have now begun to study the possibility of developing adaptive *parallel* simulation algorithms, and have begun to review and benchmark popular simulation packages (GROMACS, NAMD, OpenMM, etc.), depending on the number of atoms, the number of available cores, etc.

5.4. Protein secondary structure prediction for dynamic simulations

Participants: Marc Piuzzi, Sergei Grudinin, Stephane Redon.

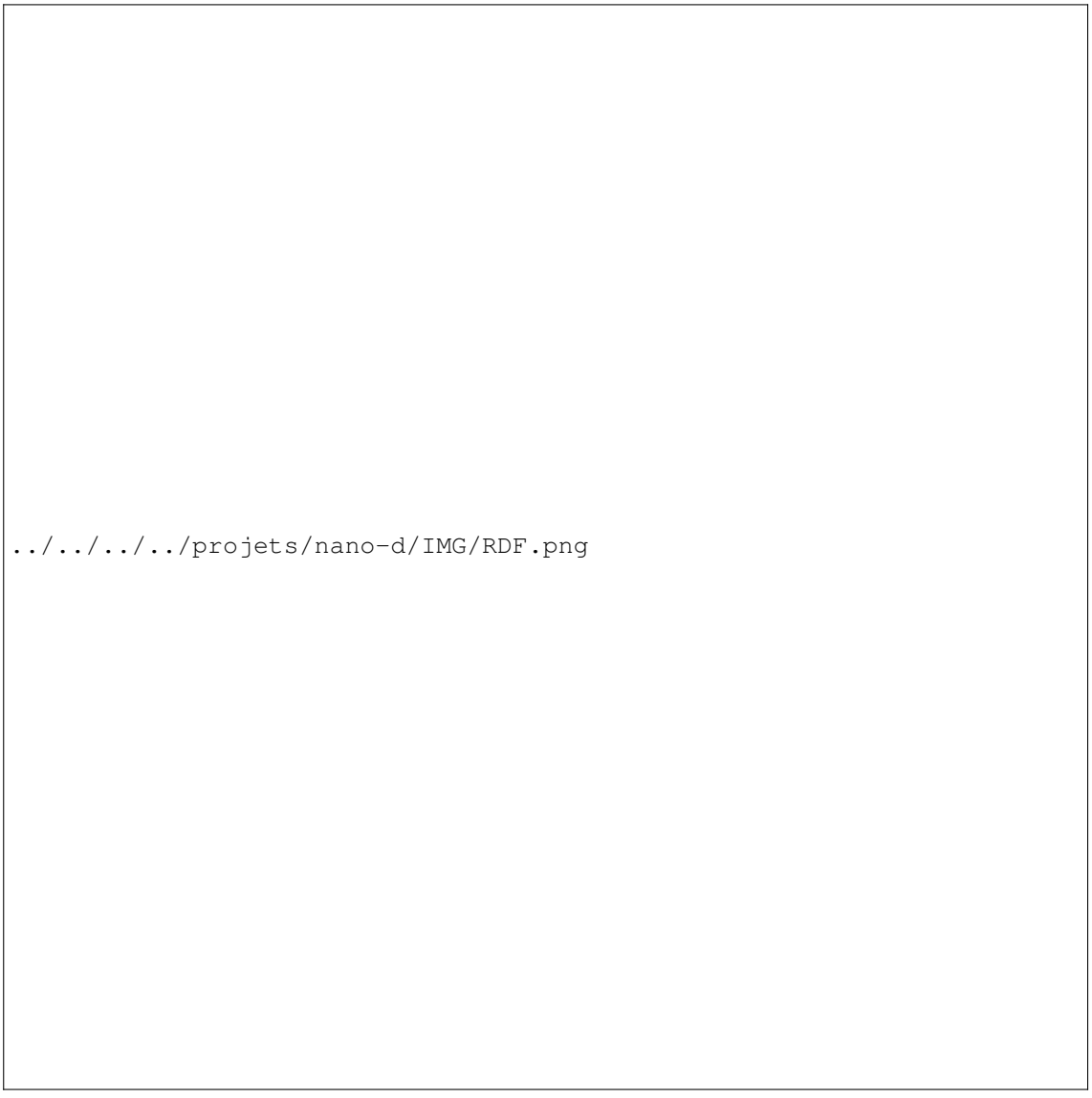


Figure 4. Radial distribution function obtained with different ARPS simulations compared to the full dynamics (blue dash line)

There is a tight link between a protein's function and its molecular structure. Hence, global stability is essential for a protein to keep its role inside the cell. Various chemical interactions helps stabilizing the structure (covalent bonds, hydrogen bonds, etc.) but not all parts of a protein present the same stability. The most stable regions of a protein present numerous hydrogen bonds on backbone atoms composing geometrically distinguishable secondary structures (the primary structure being the amino acid sequence): helices and beta sheets.

These structures have been well studied and although important properties have been defined, there is no absolute definition of what is a helix or a beta sheet. Thus, various methods have been developed to predict the secondary structure of a protein using the amino acid sequence and/or the protein structure using different parameters and structural descriptors.

However, none of these methods have been made in the context of interactive simulation where the shape of the protein is dynamic: here the prediction has to be done at each time step on the whole protein. Moreover, the result is deterministic and returns only the type of structure without any information about the accuracy. We are developing a new approach that is appropriate in an interactive context, where secondary structure assignment has to continuously change during interaction.

5.5. Motion Planning for Quasi-Static Simulation

Participants: Leonard Jaillet, Stephane Redon.

Recently, motion planning methods inspired from Robotics have been applied to the study of biological molecular systems [8]. These approaches rely on compact graph representations that aim to capture large amplitude motions more efficiently than classic simulation techniques, despite their lower resolution.

We developed within the SAMSON's architecture a new motion planning strategy to perform quasi-static simulation at the nano-scale.

The user provides as inputs the initial and final state of the system he or she wants to simulate. Then, the method searches a transition path that follows the low-energy valleys of the conformational landscape (see figure 5).

The adaptation of motion planning approaches to quasi-static simulation at the nano-scale comes with several challenges. First, these approaches must be adapted to tackle the high dimensionality involved in the case of nanosystems, dimensionality that is directly related to the number of atoms considered. Second, these approaches must be extended to face the complexity of the underlying physics that comes from the various types of interactions between atoms.

The method we propose is able to perform simulations involving bonds breaking. This is, up to our knowledge, the first motion planning approach able to simulate chemical reactions.

5.6. Molecular Modeling

5.6.1. Rapid determination of RMSDs corresponding to macromolecular rigid body motions

Participants: Petr Popov, Sergei Grudinin.

Finding the root mean sum of squared deviations (RMSDs) between two coordinate vectors that correspond to the rigid body motion of a macromolecule is an important problem in structural bioinformatics, computational chemistry and molecular modeling. Standard algorithms compute the RMSD with time proportional to the number of atoms in the molecule. We developed *RigidRMSD*, a new algorithm that determines a set of RMSDs corresponding to a set of rigid body motions of a macromolecule in constant time with respect to the number of atoms in a molecule. Our algorithm is particularly useful for rigid body modeling applications such as rigid body docking, and also for high-throughput analysis of rigid body modeling and simulation results. A C++ implementation of our algorithm will be available at http://nano-d.inrialpes.fr/software/RigidRMSD.

Figure 5. Snapshots of the transition path obtained with our motion planning simulation method. It represents a chemical reaction where two molecules of methanes interact to form a an ethane and a dihydrogen.

To demonstrate the efficiency of the RigidRMSD library, we compared the clustering application implemented with our algorithm to the one from the Hex software. We chose Hex for the comparison because it is a very fast rigid body docking tool and also because it explicitly provides the clustering time. For the comparison, we collected a small benchmark of 23 protein dimers of various size. After, we launched Hex version 6.3 on this benchmark and collected docking solutions before clustering, sizes of clusters, and clustering time. We then also clustered these solutions using the *RigidRMSD* library. Figure 6 shows the clustering time of the HEX clustering algorithm with respect to our clustering using two rotation representations as a function of the number of atoms in the smaller protein (left) and the number of docking solutions before the clustering (right). We can clearly see that our implementation of the clustering algorithm is more than an order of magnitude faster compared to the Hex implementation. Also, the quaternion representation of rotation is on average three times more efficient compared to the matrix representation.

Figure 6. Left: Time spent on clustering by Hex and RigidRMSD with respect to the number of atoms in the ligand protein. Number of considered solutions and the RMSD threshold was fixed to 10,000 and 10.0 Å, respectively. Right: Average time spent on clustering by Hex and RigidRMSD with respect to the number of docking solutions. For this plot we chose five structures with the number of atoms of about 2,000 and plotted the standard deviation of the running time. For both plots, the RMSD threshold was fixed to 10.0 Å.

5.6.2. Fast fitting atomic structures into a low-resolution density map using 3D orthogonal Hermite functions

Participants: Georgy Derevyanko, Sergei Grudinin.

We developed a new algorithm for fitting protein structures into a low resolution electron density (e.g. cryo-electron microscopy) map. The algorithm uses 3D orthogonal Hermite functions for fast operations on the electron density.

Orthogonal Hermite function of order n is defined as:

$$\psi_n(x;\lambda) = \frac{\sqrt{\lambda}}{\sqrt{2^n n!\sqrt{\pi}}} \exp\left(-\frac{\lambda^2 x^2}{2}\right) H_n(\lambda x), \tag{1}$$

where $H_n(x)$ is the Hermite polynomial and λ is the scaling parameter. In Fig. 7 we show several orthogonal Hermite functions of different orders with different parameters λ. These functions form an orthonormal basis set in $L^2(\mathbb{R})$. A 1D function $f(x)$ decomposed into the set of 1D Hermite functions up to an order N reads

$$f(x) = \sum_{i=0}^{N} \widehat{f}_i \psi_i(x;\lambda) \tag{2}$$

Here, $\widehat{f}_i$ are the decomposition coefficients, which can be determined from the orthogonality of the basis functions $\psi_i(x;\lambda)$. Decomposition in Eq. 2 is called the *band-limited decomposition* with $\psi_i(x;\lambda)$ basis functions. To decompose the electron density map and the protein structures, we employ the 3D Hermite functions:

$$\psi_{n,l,m}(x,y,z;\lambda) = \psi_n(x;\lambda)\psi_l(y;\lambda)\psi_m(z;\lambda), \tag{3}$$

which form an orthonormal basis set in $L^2\left(\mathbb{R}^3\right)$. A function $f(x,y,z)$ represented as a band-limited expansion in this basis reads

$$f(x,y,z) = \sum_{i=0}^{N} \sum_{j=0}^{N-i} \sum_{k=0}^{N-i-j} \widehat{f}_{i,j,k} \psi_{i,j,k}(x,y,z;\lambda) \tag{4}$$

Our algorithm accelerates rotation of the Fourier image of the electron density by using 3D orthogonal Hermite functions. As a part of the new method, we presented an algorithm for the rotation of the density in the Hermite basis and an algorithm for the conversion of the expansion coefficients into the Fourier basis. We implemented the program of fitting a protein structure to a low-resolution electron density map, which uses the cross-correlation or the Laplacian-filtered cross-correlation as the fitting criterion. We demonstrated that in the Hermite basis, the Laplacian filter has a particularly simple form. To assess the quality of density encoding in the Hermite basis, we uses two measures, the R-factor and the cross-correlation factor. Finally, we validated our algorithm using two examples and compare its efficiency with two widely used fitting methods, ADP_EM and *colores* from the Situs package.

5.6.3. Fast Rotational-Translation Matching of Rigid Bodies by Fast Fourier Transform Acceleration of Six Degrees of Freedom

Participants: Alexandre Hoffmann, Sergei Grudinin.

We introduced a new method for rigid molecular fitting. This problem is usually solved by maximizing the Cross Corelation Function (CCF), which is computed using the Fast Fourier Transform (FFT) algorithm. Our method handles six degrees of freedom at once and requires only one computation of the Cross Corelation Function, with the six-dimensional Fast Fourier Transform. Our method only requires a low pre-processing time ($O(N^7)$), which is comparable to the cost of the subsequent 6D FFT ($O(N^6 \log(N^6))$). It also uses a dual Hermite-Fourier representation, which allows to represent a small molecule with a fewer number of coefficients in the Hermite basis.

5.6.4. Prediction of complexes with point group symmetry using spherical polar Fourier docking correlations

Participants: David W. Ritchie, Sergei Grudinin.

Many proteins form symmetric homo-oligomers that perform a certain physiological function. We present the first point group symmetry docking algorithm that generates perfectly symmetrical protein complexes for arbitrary point group symmetry types (C_n, D_n, T, O, and I). We validate the algorithm on proteins from the 3D-Complex database, where it achieves on average the success rate of 55%. The running time of the algorithm is less than a minute on a modern workstation.

Figure 7. Left: 1D Hermite functions of order 6 for three different scaling parameters λ. Right: 1D Hermite functions of two different orders for the scaling parameter $\lambda = 1$.

Many of the protein complexes in the protein Data bank (PDB) are symmetric homo-oligomers. According to the 3D-Complex database, C_2 homo-dimers comprise the majority of known homo-oligomers. However, many complexes have higher order rotational symmetry (i.e. C_n>2), and a good number have multiple rotational symmetry axes, namely those with dihedral (D_n), tetrahedral (T), octahedral (O), and icosahedral (I) point group symmetries. Although symmetrical complexes are often solved directly by X-ray crystallography, it would still be very useful to be able to predict whether or not a given monomer might self-assemble into a symmetrical structure. We present a new point group symmetry docking algorithm. In the last few years, several protein-protein docking programs have been adapted to predict symmetrical pair-wise docking orientations for C_n and D_n symmetries. However, to our knowledge, there does not yet exist an algorithm which can automatically generate perfectly symmetrical protein complexes for arbitrary point group symmetry types.

We introduce the notion of a "docking equation" in which the notation $A(\underline{x}) \longleftrightarrow B(\underline{x})$ represents an interaction between proteins A and B in 3D space. It is also useful introduce the operators $\widehat{T}(x, y, z)$ and $\widehat{R}(\alpha, \beta, \gamma)$, which represent the actions of translating an object by an amount (x, y, z) and rotating it according to the three Euler rotation angles (α, β, γ). Then, guided by Figure 8 , and assuming that we start with two identical monomers at the origin, we can write down a C_n docking equation for the two monomers as

$$\widehat{T}(0, y, 0)\widehat{R}(\alpha, \beta, \gamma)A(\underline{x}) \longleftrightarrow \widehat{R}(0, 0, \omega)\widehat{T}(0, y, 0)\widehat{R}(\alpha, \beta, \gamma)B(\underline{x}). \tag{5}$$

Then, we perform a series of fast Fourier transform (FFT) correlation searches using the Hex spherical polar Fourier docking algorithm to determine the four parameters $(y, \alpha, \beta, \gamma)$. For higher symmetries, D_n, T, O, and I, we introduce two more parameters and perform a series of FFT in a similar way. The calculation for each structure takes less than a minute on a modern workstation.

Figure 8. Illustrations of the C_3 and D_3 point group symmetries.

We validated our method on protein structures from the 3D-Complex database, which contains 17,183 protein complexes with assigned biological unit and symmetry type. It mostly contains cyclic and dihedral proteins, as well as 86 tetrahedral, 47 octahedral, and 6 icosahedral complexes (excluding all viral structures). Starting

from the structures of monomers, we generated symmetric biological units based on the symmetry type for each complex provided by 3D-Complex. Figure 9 summarizes the performance of our method on these proteins, where we say that the model is correct if all pair-wise RMSDs are smaller than 10 Ångstroms. On average, we found about 55% of correct predictions ranked first.

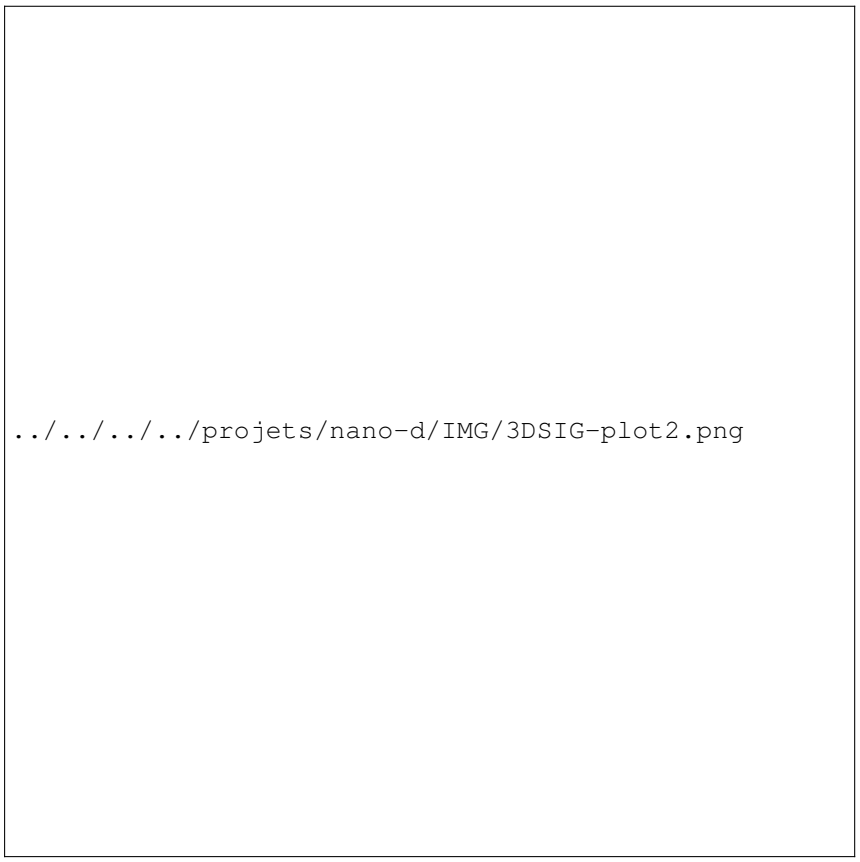


Figure 9. Summary of the correctly predicted complexes found on the first place (blue) and in the top ten solutions (green).

Figure 10 shows correctly predicted examples from each of the symmetry types. Each complex is perfectly symmetrical, although due to the soft docking function in Hex it is possible that some interfaces might contain minor steric clashes.

5.7. Software Engineering

5.7.1. SAMSON User interface

Participants: Jocelyn Gate, Maria Werewka, Stephane Redon.

We have continued the development of SAMSON, our open-architecture platform for modeling and simulation of nanosystems (SAMSON: Software for Adaptive Modeling and Simulation Of Nanosystems):

- We have moved to Qt5 to handle the Graphical User Interface.

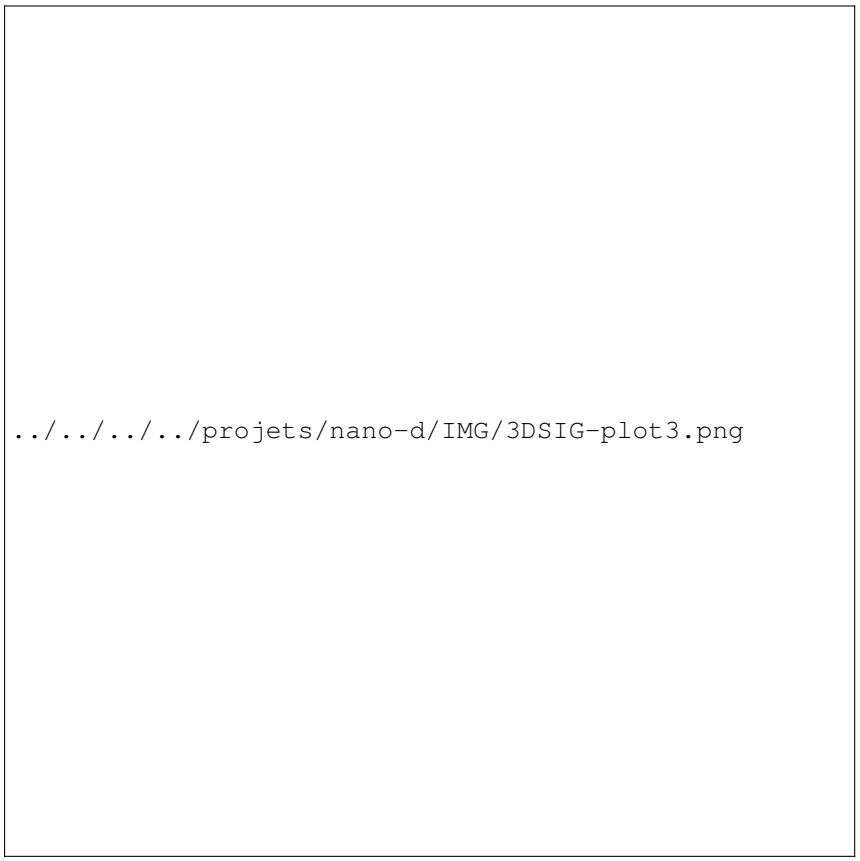


Figure 10. Illustrations of the correctly predicted complexes. For each complex, the group symbol and the PDB code are shown.

- We now compile SAMSON is 64 bits only. This removes limitations of 32 bits applications, in particular concerning memory limits.
- We now have a complete installer mechanism for both users and developers.
- We extended the set of development tools (action generators, UUID generators, etc.)
- We have changed the windowing system to allow windows to move outside SAMSON.
- We have designed a coherent style for icons, windows, menus, etc.
- We have added 3D rendering.

There are now more than 40 modules in SAMSON (parsers, editors, models, apps, etc.).

The current user interface of SAMSON is visible in Figure 11 .

5.7.2. SAMSON Elements

Participants: Svetlana Artemova, Stephane Redon.

We have added new SAMSON Elements (modules).

We have been working on input and output for SAMSON. Precisely, we now have the possibility to download molecules to SAMSON and save them to external files in three possible formats:

- pdb (Protein Data Bank format, containing experimentally determined 3d structures and widely used for applications in biology);
- mol2 (Sybyl chemical modeler input file, containing chemical compounds and small ligands);
- xyz (basic format, containing atoms coordinates).

Basic properties of atoms, residues, and molecules have been determined and structures storing these properties were implemented.

Finally, since energy minimization is crucial for providing physically-correct structures while interactively editing molecules in SAMSON, we have implemented several fast and stable algorithms to perform such energy minimization in SAMSON.

5.7.3. SAMSON Website

Participants: Mohamed Yengui, Jocelyn Gate, Stephane Redon.

We are developing a web application aiming at distributing and valorizing SAMSON and SAMSON Elements (modules). The goal of the website is to develop a community of users and developers in all areas of nanoscience (physics, biology, chemistry, electronics, etc.). The website will:

- allow users and developers to create and manage accounts on the website.
- allow visualizing, searching and downloading SAMSON and SAMSON Elements.
- allow the creation, validation and dissemination of SAMSON Elements.
- provide tracking requests for the arrival of new SAMSON Elements or the modification of an existing SAMSON Element.

To achieve this, we have designed the architecture in a way that speeds development effort for a faster product release, while keeping in mind scalability, security and high reliability.

We have also implemented and tested locally the account validation process. A user can now sign up, confirm the registration from the received email and authenticate with the registered account to download SAMSON and SAMSON elements from the website. We will make the site public when we release SAMSON.

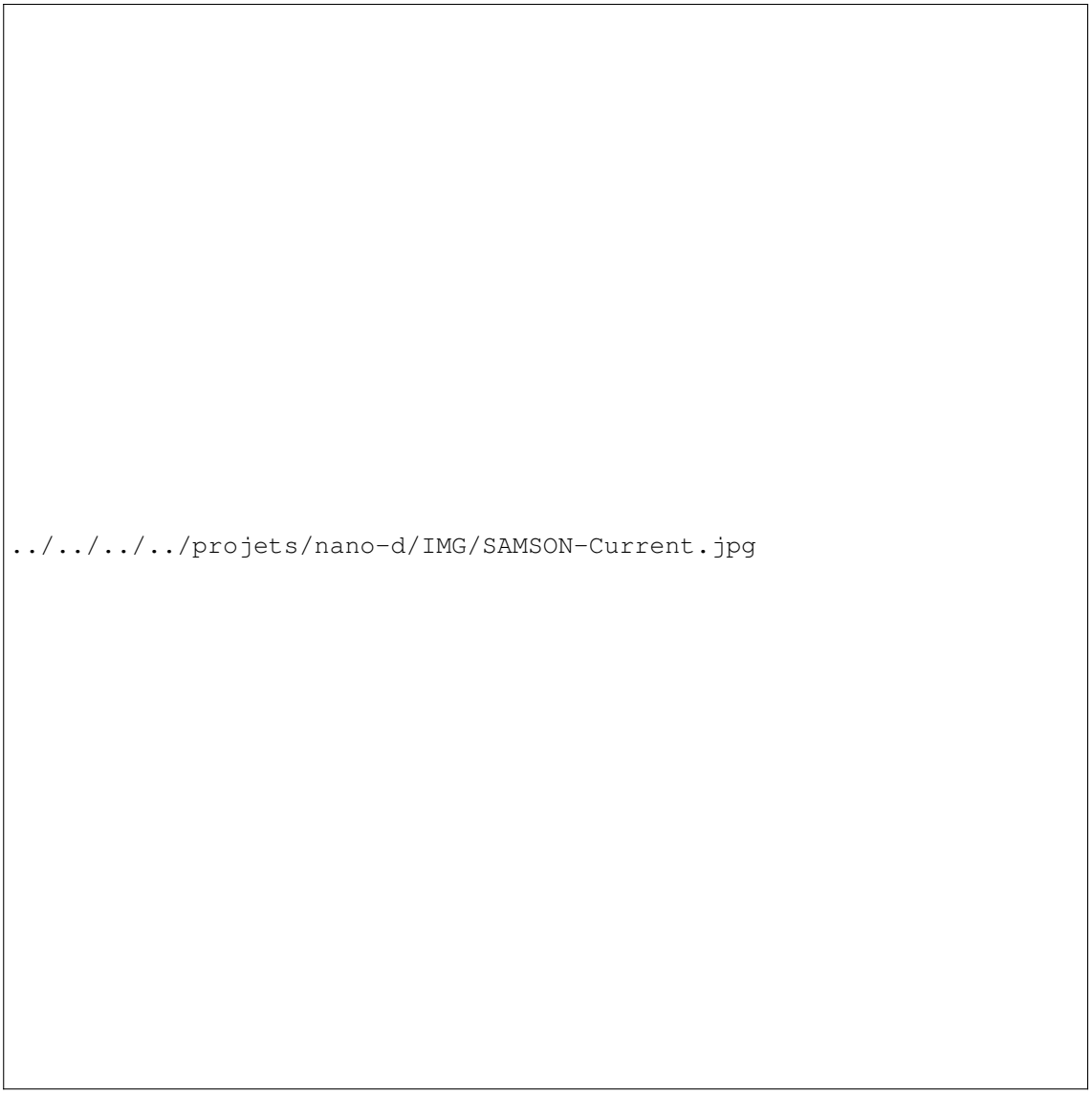


Figure 11. The current user interface of SAMSON showing an app to download molecules directly from the Protein Data Bank. The data graph on the left shows the hierarchical structure of the structural model.

OPALE Project-Team

6. New Results

6.1. Mathematical analysis and control of macroscopic traffic flow models

6.1.1. Vehicular traffic

Participants: Alessandra Cabassi, Maria Laura Delle Monache, Paola Goatin, Alexandre Bayen [UC Berkeley, CA, USA], Legesse Lemecha Obsu [Addis Ababa University, Ethiopia].

In collaboration with UC Berkeley, and as part of the Associated Team ORESTE activity (see http://www-sop.inria.fr/members/Paola.Goatin/ORESTE/index.html), we have proposed a new junction model for ramp metering: we introduce a coupled PDE-ODE model, in which the PDE describes the evolution of the cars flow on the main lane and the ODE describes the evolution of the queue length on the on-ramp, modeled by a buffer, which ensures that boundary conditions are satisfied in strong sense. We were able to prove existence and uniqueness of the solution of the corresponding Riemann problem [41]. Relying on the above junction model, we have applied the Discrete Adjoint Method to efficiently compute (locally) optimal ramp-metering parameters to minimize the total travel time on a stretch of highway [80].

In parallel, we have proposed two optimization strategy for instantaneous optimization of total travel times and total waiting times at roundabouts, which give an estimate of the time spent by drivers on the network section. These cost functionals are minimized with respect to the right-of-way parameter of the incoming roads. For each cost functional, the analytical expression is given for each junction, see [72]. This work is part of L.L. Obsu's PhD thesis.

Finally, we designed a new finite volume algorithm to track the trajectory of a bus in the surrounding traffic using a locally non-uniform moving mesh, see [3, 4, 5].

As part of our TRAM3 activity, we also organized the workshop "TRAM2 - Traffic Modeling and Management: Trends and Perspectives", which successfully took place at Inria Sophia Antipolis on March 20-22, 2013 (see https://team.inria.fr/opale/workshop-tram2/).

In the framework of the EIT ITC Labs Multimodal Mobility activity, A. Cabassi's internship was devoted to the calibration and the validation of a first order traffic flow model against processed real data provided by the industrial partners Autoroutes Traffic and VINCI Autoroutes, see [69].

6.1.2. Crowd motion

Participants: Régis Duvigneau, Paola Goatin, Matthias Mimault, Debora Amadori [L'Aquila University, Italy], Christophe Chalons [LJLL, UP7], Massimiliano D. Rosini [ICM, Warsaw University, Poland], Nicolas Seguin [LJLL, UPMC], Monika Twarogowska.

From the analytical point of view, we have been studying the properties of some models in one space dimension. Concerning Hughes' scalar model, we have established a partial existence result in collaboration with D. Amadori and M.D. Rosini (see [75]). M. Mimault's internship in 2012 was devoted to develop a MATLAB code based on wave-front tracking to compute the solutions of Hughes' model with generalized running cost, see [42]. He is currently working on a mixed hyperbolic-elliptic 2x2 system of conservation laws describing two groups of people moving in opposite directions. Finally, in collaboration with C. Chalons and N. Seguin, we generalized previous results on conservation laws with local flux constraints [3], [5] to general flux functions and non-classical solutions arising in pedestrian flow modeling, see [39]. From the numerical point of view, we have implemented some macroscopic models in 2D on unstructured triangular meshes on the Num3sis platform. We provided a comparison between first and second order models in reproducing complex dynamics of crowd motion, such as formation of stop-and-go waves and clogging at bottlenecks. Then, we concentrated on the higher-order model and analyzed the dependence of the behavior of its solutions on some of the parameters of the system. In particular, we produced some examples where placing obstacles in front of the door prevents from blocking and decreases the evacuation time, see [73], [81].

The above researches were partially funded by the ERC Starting Grant "TRAM3 - Traffic management by macroscopic models".

6.2. Optimum design and control in fluid dynamics and its couplings

In computational sciences for physics and engineering, Computational Fluid Dynamics (CFD) are playing one of the major roles in the scientific community to foster innovative developments of numerical methodologies. Very naturally, our expertise in compressible CFD has led us to give our research on numerical strategies for optimum design a particular, but not exclusive focus on fluids.

The framework of our research aims to contribute to numerical strategies for PDE-constrained multi-objective optimization, with a particular emphasis on CPU-demanding computational applications in which the different criteria to be minimized (or reduced) originate from different physical disciplines that share the same set of design variables. These disciplines are often fluids, as a primary focus, coupled with some other disciplines, such as structural mechanics.

Our approach to *competitive optimization* is focused on the two-discipline problem. It is based on a particular construction of *Nash games*, relying on a *split of territory* in the assignment of individual strategies. A methodology has been proposed for the treatment of two-discipline optimization problems in which one discipline, the primary discipline, is preponderant, or fragile. Then, it is recommended to identify, in a first step, the optimum of this discipline alone using the whole set of design variables. Then, an orthogonal basis is constructed based on the evaluation at convergence of the Hessian matrix of the primary criterion and constraint gradients. This basis is used to split the working design space into two supplementary subspaces to be assigned, in a second step, to two virtual players in competition in an adapted Nash game, devised to reduce a secondary criterion while causing the least degradation to the first. The formulation has been proved to potentially provide a set of Nash equilibrium solutions originating from the original single-discipline optimum point by smooth continuation, thus introducing competition gradually [53]. (see also subsectionsubsect:helico).

Our approach to *cooperative optimization*, in theory, is not limited in number of objective functions. It is based on a result of convex analysis established for a general unconstrained mult-iobjective problem in which all the gradients are assumed to be known. The theorem [16] states that in the convex hull of the gradients, there exists a unique vector of minimal norm, ω; if it is nonzero, the vector ω is a descent direction common to all criteria; otherwise, the current design point is Pareto-stationary. This result led us to generalize the classical steepest-descent algorithm by using the vector ω as search direction. We refer to the new algorithm as the multiple-gradient descent algorithm (MGDA). The MGDA yields to a Pareto-stationary point, and actual Pareto-optimality is then tested [54] (see also subsection 6.2.4).

The two approaches have been combined to explore the Pareto front segment-wise as illustrated on Figure 2 .

6.2.1. Multiple-Gradient Descent Algorithm (MGDA)

Participants: Jean-Antoine Désidéri, Régis Duvigneau, Matteo Giacomini, Abderrahmane Habbal, Adrien Zerbinati.

6.2.1.1. Theory and numerical experimentation of the MGDA construction

In multi-objective optimization, the knowledge of the Pareto set provides valuable information on the reachable optimal performance. A number of evolutionary strategies (PAES, NSGA-II, etc), have been proposed in the literature and proved to be successful to identify the Pareto set. However, these derivative-free algorithms are very demanding in terms of computational time. Today, in many areas of computational sciences, codes are developed that include the calculation of the gradient, cautiously validated and calibrated.

The notion of Pareto-stationarity, originally established to be a necessary condition of optimality in differentiable multi-objective optimization of unconstrained problems, has been extended to problems subject to equality constraints. On this basis, we were able to establish that by augmenting, in a classical manner, the objective-functions of a penalty term equal to the square of the constraint violation, and applying the standard MGDA to it, would result in converged solutions that are Pareto-stationary in the extended sense. Numerical experimentation on this is on-going.

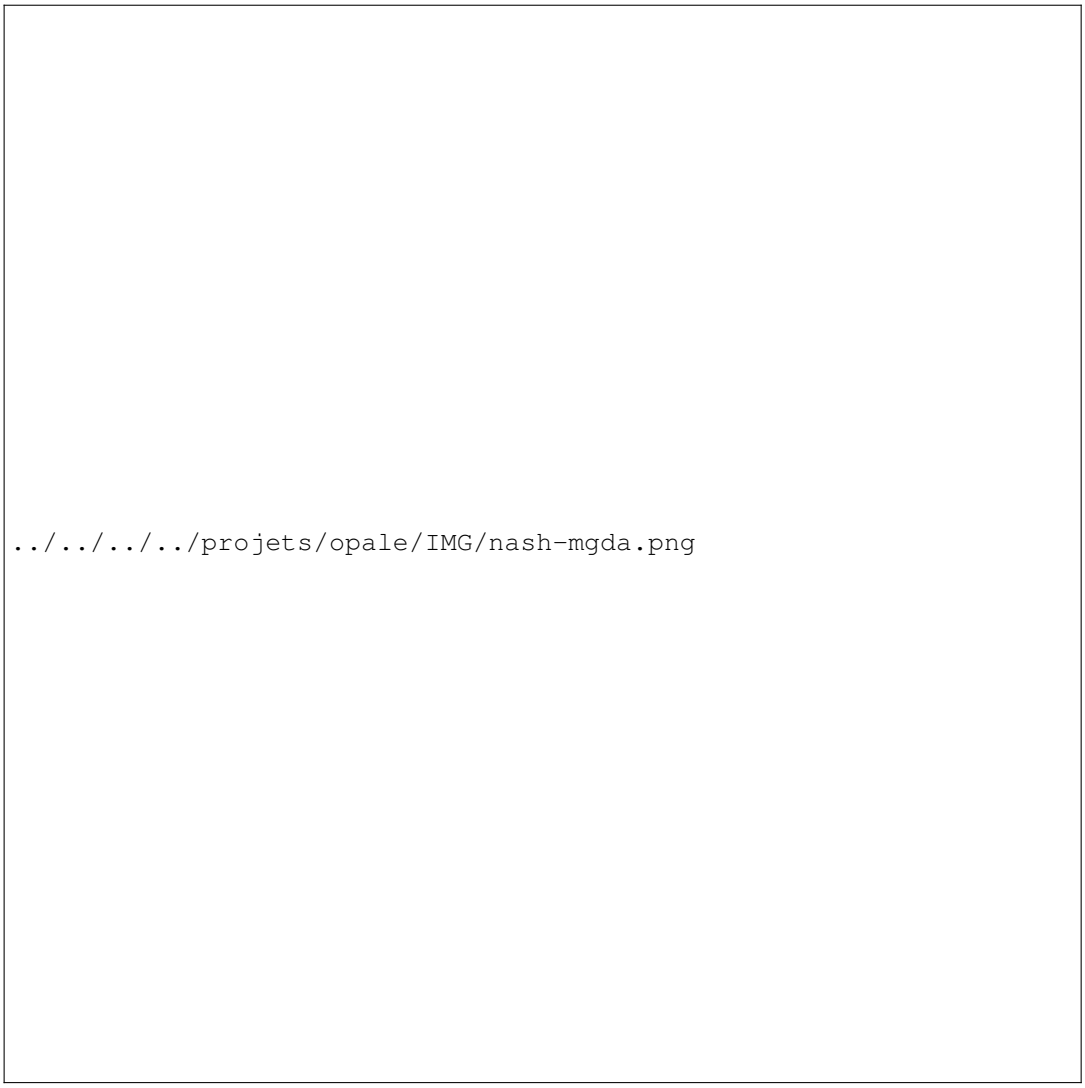


Figure 2. ***Two-discipline optimization of a generic geometry of a supersonic aircraft, for concurrent drag and sonic-boom reduction*** *(from A. Minelli's doctoral thesis). The wave drag is calculated by the ONERA elsA code in 3D finite-volume Eulerian flow mode over a 6M-node mesh and the sonic boom using a three-layer approach. The Nash-game paths have been devised by appropriate territory splitting in order to be tangent to the Pareto front, and they are interrupted whenever the Pareto-stationarity condition is judged excessively violated. The MGDA paths converge rapidly back to the front. The simulation demonstrates how the two algorithms complement each other and provide a potential for a piecewise description of the Pareto front, evaluated more economically than a stochastic algorithm operating on a large population.*

6.2.1.2. Meta-model-assisted CFD optimization by MGDA

Using MGDA in a multi objective optimization problem requires the evaluation of a large number of points with regard to criteria, and their gradients. In the particular case of a CFD problems, each point evaluation is very costly since it involves a flow computation, possibly the solution of an adjoint-equation. To alleviate this difficulty, we have proposed to construct meta-models of the functionals of interest (lift, drag, etc) and to calculate approximate gradients by local finite differences. These meta-models are updated throughout the convergence process to the evaluation of the new design points by the high-fidelity model, here the 3D compressible Euler equations.

This variant of MGDA has been tested successfully over a problem of external aerodynamic optimum-shape design of an aircraft wing consisting of reducing wave-drag, and augmenting lift. After only a few cycles of database updates, the Pareto front visibly forms, and this result is achieved at a very moderate computational cost [68]. This variant has been extended successfully to an internal flow optimization problem related to an automobile air-conditioning system and governed by the Navier-Stokes equations. This more difficult problem has been proposed by Renault within the OMD2 ANR project. These studies have been reported in A. Zerbinati's doctoral thesis [38].

6.2.1.3. Exact shape gradients

MGDA has successfully been tested over a two-objective optimization problem governed by two-dimensional elasticity. The deformation of a plate is calculated using an isogeometric approximation (see 6.3) and compliance derived from it. The exact parametric shape gradient is calculated, yielding the gradient of the objective function in two antagonistic situations differing by the loading. Pareto-fronts are thus identified.

6.2.1.4. Perspectives

MGDA offers the possibility to handle in a rational way several objective-functions for which gradients are known or approximated concurrently. This potential opens methodological paths to several themes of interest in high-fidelity simulation-based optimization: optimization of complex systems whose performance is evaluated w.r.t. several criteria originating from different, coupled disciplines; optimization under uncertainties, by introducing sensitivities as additional objectives; optimization of time-dependent systems, such as optimization of flow-control devices that generate a periodic flow (see next subsection), by converting the problem into a multi-point problem by time-discretization of the time and parameter-dependent functional; etc.

6.2.2. Flow control

Participants: Régis Duvigneau, Jérémie Labroquère, Emmanuel Guilmineau [Ecole Centrale de Nantes].

Shape optimization methods are not efficient to improve the performance of fluid systems, when the flow is characterized by a strong unsteadiness related to a massive detachment. This is typically the case for the flow around an automotive body or a wing in stall condition. To overcome this difficulty, flow control strategies are developed, that aim at manipulating vortex dynamics by introducing some active actuators, such as periodic blowing/suction jets. In this context, the choice of the control parameters (location, amplitude, frequency) is critical and not straightforward. Therefore, we develop a methodology to determine optimal control parameters by coupling the simulation of unsteady actuated flows with optimization algorithms. Two research axes have been considered :

- the resolution of the unsteady sensitivity equations derived from the state equations, to exhibit the dependency of the flow dynamics with respect to the control ;
- the optimization of control parameters using a statistical metamodel-based strategy.

In this perspective, unsteady Reynolds Averaged Navier-Stokes equations are solved, with some turbulence closures. Different models for synthetic jet have been implemented to simulate the actuation, and then validated for different turbulence closures [70].

Specific developments have be carried out in the metamodel-based optimizer to include a noise term into Gaussian Process model, which is used to filter errors arising from unsteady simulations. A systematic assessment of modeling and numerical errors has been archived [57], for a backward facing step test-case, with the objective of controlling the re-attachment point location.

This activity is conducted in collaboration with the CFD team of Ecole Centrale de Nantes.

6.2.3. Robust design

Participants: Jean-Antoine Désidéri, Régis Duvigneau, Daïgo Maruyama.

This work aims at developing robust design tools for aircraft w.r.t. aerodynamic performance subject to uncertainties, arising from geometrical features and fluctuations of inflow conditions. The robust design process is considered as a multi-objective optimization problem, which consists in minimizing or maximizing statistical moments of the cost function.

In the context of airfoil design, MGDA is used to improve simultaneously the mean and variance of the lift and drag coefficients, yielding a four-objective optimization problem [71].

6.2.4. Sonic boom reduction

Participants: Gérald Carrier [Research Engineer, ONERA/DAAP], Jean-Antoine Désideri, Andrea Minelli, Itham Salah El Din [Research Engineer, ONERA/DAAP].

When an aircraft flies at supersonic speed, it generates at ground level an N-shaped shock structure which can cause serious environmental damage ("sonic boom"). Thus a problem of interest in aerodynamic optimization is to design such an aircraft to reduce the intensity of the sonic boom while maintaining the aerodynamic performance (drag minimization under lift constraint). Andrea Minelli aimed at contributing to this two-discipline optimization problem. In the first part of his work, an inverse problem has been formulated and solved for "shaped sonic boom" and found in excellent agreement with the George-Seebass-Darden theory [82] for the calculation of the Whitham function corresponding to the lowest-boom (axisymmetric) shape. Method and results have been generalized to more general geometries and have been presented internationally in [58].

Besides, aero-acoustic optimizations have been realized successfully by coupling the aerodynamic optimizer (based on Euler calculations by the elsA software) with the sonic-boom computation in a Nash game formulation. These experiments, conducted with our optimization platform FAMOSA, have demonstrated that starting from the shape optimized aerodynamically, one could retrieve smoothly a shape corresponding to nearly-optimal sonic-boom reduction [36]. and [54].

6.2.5. Helicopter rotor blade optimization in both situations of hovering and forward flight

Participants: Michel Costes [Research Engineer, ONERA/DAAP], Jean-Antoine Désideri, Arnaud Le Pape [Research Engineer, ONERA/DAAP], Enric Roca Leon.

E. Roca Leon is conducting a CIFRE thesis supported by EUROCOPTER (Marignane) at ONERA DAAP. This thesis follows the doctoral thesis of A. Dumont in which the adjoint-equation approach was used to optimize a rotor blade in hovering flight. The goal of this new thesis is to solve a two-objective optimization problem in which the hovering-flight criterion is considered preponderant, but a new criterion that takes into account the forward-flight situation is also introduced, concurrently. The second criterion is the power necessary to maintain the forward motion. The first phase of thesis work has been devoted to the set up of a hierarchy of models from low to high fidelity, in order to calibrate appropriate functional criteria. Then, actual two-objective optimizations are conducted via our Nash game approach to competitive optimization with territory splitting based on reduced Hessian diagonalization. A first successful experiment has been realized in which 16 geometrical parameters have been optimized to reduce the power in forward motion while maintaining sub-optimality of the drag in hover. These results have been accepted for presentation at the American Helicopter Society Forum [62], and [53].

6.2.6. Optimum design in naval hydrodynamics

Participants: Régis Duvigneau, Louis Blanchard, Elisa Berini [K-Epsilon company].

Naval hydrodynamics field has recently shown a growing interest for optimum design methods. The computational context is especially complex because it implies unsteady two-phase turbulent flows, with possibly very high Reynolds number (up to 10^9). The use of automated design optimization methods for such problems requires new developments to take into account the large CPU time necessary for each simulation and the specificity of the geometries considered.

Some developments have been initiated on the geometrical modelling of hull shapes by parametric surfaces. The objective was to be able to modify existing hull shapes by controlling a small number of parameters, that are meaningful for naval architects. We have considered as test-case the bow shape for trawler ships. As a second step, an optimum shape procedure has been set up, based on a metamodel-based optimizer, the developed CAD model and the simulation tool for free-surface flows provided by K-Epsilon company. The objective was to reduce the wave drag of a trawler ship by adding a bow, whose parameters are optimized [50].

6.3. Isogeometric analysis and design

Participants: Régis Duvigneau, Bernard Mourrain [Galaad project-team], Alexandros Ginnis [Nat. Tech. Univ. of Athens], Bernd Simeon [Tech. Univ. of Kaiserslautern], Gang Xu [Hangzhou Dianzi Univ.].

Design optimization stands at the crossroad of different scientific fields (and related software): Computer-Aided Design (CAD), Computational Fluid Dynamics (CFD) or Computational Structural Dynamics (CSM), parametric optimization. However, these different fields are usually not based on the same geometrical representations. CAD software relies on Splines or NURBS representations, CFD and CSM software uses grid-based geometric descriptions (structured or unstructured), optimization algorithms handle specific shape parameters. Therefore, in conventional approaches, several information transfers occur during the design phase, yielding approximations that can significantly deteriorate the overall efficiency of the design optimization procedure. Moreover, software coupling is often cumbersome in this context.

The isogeometric approach proposes to definitely overcome this difficulty by using CAD standards as a unique representation for all disciplines. The isogeometric analysis consists in developing methods that use NURBS representations for geometric modeling, computational domain description and solution basis functions. Using such a unique data structure allows to compute the solution on the exact geometry (not a discretized geometry), obtain a more accurate solution (high-order approximation), reduce spurious numerical sources of noise that deteriorate convergence, avoid data transfers between the software. Moreover, NURBS representations are naturally hierarchical and allows to define multi-level algorithms for solvers as well as optimizers.
In this context, some studies on elliptic problems have been conducted in collaboration with the Galaad project-team and Hangzhou Dianzi University, such as the development of methods for adaptive parameterization including an a posteriori error estimate [46], [47], [48]. A collaborative work has also been carried out with the Technical University of Kaiserslautern, concerning the computation of shape gradients for linear elasticity problems, and with the National Technical University of Athens for hull shape optimization [55].

6.4. Optimum design in structural mechanics

6.4.1. Shape Optimization in Multidisciplinary Non-Linear Mechanics

Participants: Aalae Benki, Jean-Antoine Désidéri, Abderrahmane Habbal, Gael Mathis [ArcelorMittal, CRAA].

In collaboration with the ArcelorMittal's Center for Research in Automotive and Applications (CRAA), we study the multidisciplinary shape and parameter design of highly non linear mechanical 2D and 3D structures. We have developed methods adapted to the approximation of Pareto Fronts such as Normal Boundary Intersection NBI and Normalized Normal Constraint Method NNCM. Due to the time consuming cost evaluation, the use of cheap to evaluate surrogate models is mandatory. We have studied the consistency of the approach NBI or NNCM plus surrogates, which turned out to be successful for a broad panel of standard mathematical benchmarks. The coupling is successfully applied to a small scale industrial case, namely the shape optimization of a can bottom vis à vis dome reversal pressure and dome growth criteria. We have

then defined a Nash game between criteria where the latter are approximated by the RBF metamodels. First, we validated the computation of a Nash equilibrium for mathematical functions, then we computed Nash equilibria for the small scale industrial case of the shape optimization of the can bottom.

Then, we considered the 3D problem of an automotive twist beam. In this 3D case, we aim to Pareto-optimal shapes for two objectives, the first being to minimize the Von-Mises strain to guarantee the formability of the twist beam, and the second being to maximize the stiffness. For solution with higher stiffness than the initial one, we could decrease the thickness to obtain a mass reduction with the same end-user properties.

We also introduced, to our knowledge for the first time in the structural optimization area, the notion of Kalai-Smorodinky equilibria which is aimed at the selection of equilibria among Pareto-optimal solutions. We applied this notion of equilibria to both industrial cases, and compared the results to Nash equilibria. [56] [64]

Figure 3. Concurrent design in industrial applications. A packaging problem of commercial cans (left). Automotive twist beam (right)

6.4.2. Optimization of Addendum Surfaces in Stamping

Participants: Fatima Zahra Oujebbour, Rachid Ellaia, Abderrahmane Habbal, Ziheng Zhao.

Within the OASIS Consortium (ArcelorMittal, ErDF, Inria, UTC, EURODECISION, ESILV, NECS, Delta-CAD, SCILAB-DIGITEO), the Opale project-team leads the Optimization task. Our aim is to develop decentralized decision-making algorithms dedicated to find efficient solutions (Pareto optimal) in a complex multi-disciplinary framework (forming, stamping, welding non-linear processes, spring-back, vibration, in-function linear processes, crash and fatigue non linear and non differentiable processes) for several (between three and five) criteria. An important difficulty when trying to identify the Pareto Front, even when using adapted methods such the Normal Boundary Intersection, is that the criteria involved (thanks to the high nonlinearity in the mechanical models) exhibit many local optima. So one must use global optimization methods. We have studied the hybrid approach Simulated Annealing with Simultaneous Perturbation SASP for a suite of mathematical test-cases. To envisage the application of our method to the complex CPU time consuming stamping process, we lead an intermediate phase dedicated to the validation of the SASP method for the minimization of the spring-back that follows the stamping of a metal sheet, the design variable being the process parameters (two then four parameters). Then, we considered the more complex shape design of the initial blank. The initial

blank design is a critical step in stamping design procedure, therefore it should be optimally designed. Our aim is to find the optimal initial blank shape that avoids or at least minimizes the springback and failure flaws. For this study, the geometry of the blank contour is described by parametric spline curves. Seven control points (P1,...,P7) are used to define the spline curves in order to have a wide variety of geometries. The exact computational evaluation of our criteria, springback and failure, is very expensive (the FE model request around 45 min to predict these two criteria) and the design space is of quite high dimension. Therefore, we considered the recourse to the sparse grid interpolation. Optimization process based on sparse grid interpolation is an optimal alternative in which criteria can be approximated with a suitable interpolation formula that needs significantly less points than the full grid. the obtained metamodel using sparse grid interpolation needs less than 1s to predict springback and failure on the same computation machine. To find the optimal initial blank shape, it was decided to perform the optimization process using the obtained metamodel. The construction of the sparse grid interpolant was based on the Chebyshev Gauss-Lobatto grid type and using the polynomial basis functions. This technique achieves a good accuracy with a competitive number of grid points. The comparison of the obtained fronts shows that we can capture Pareto solutions by NBI and NNCM with fewer points than NSGAII which requires a large number of populations and several generations to obtain the Pareto front. [60] [61] [63] [77]

Figure 4. Multiobjective design of the stamping process of a high performance steel sheet. The design variable is the initial blank shape, and the costs are elastic spring-back and failure. Sparse grid approximation of the costs is used. The Pareto front obtained by NBI and NNCM (lower-left) are compared to a NSGA-II one (lower-right).

6.5. Application of shape and topology design to biology and medicine

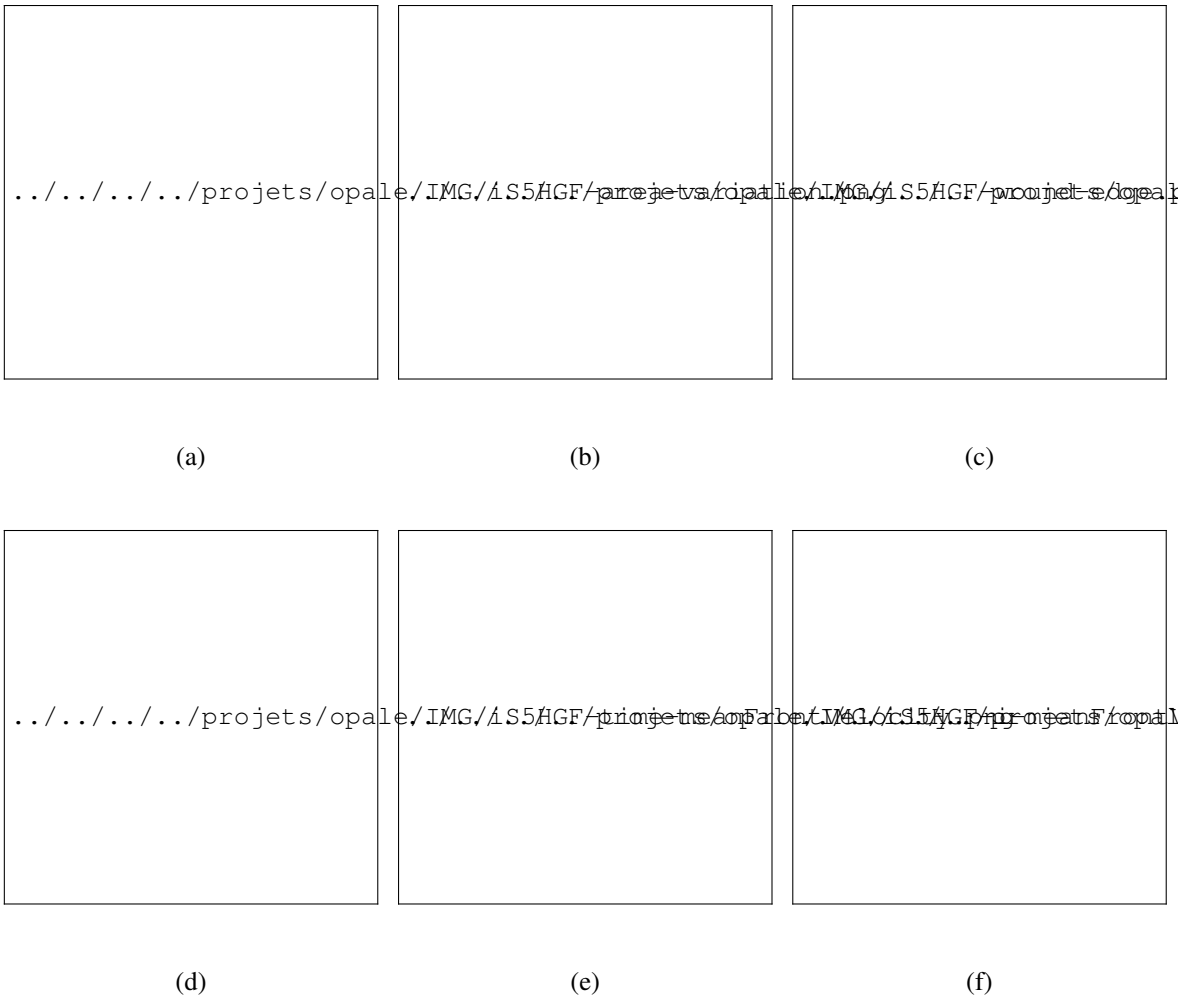
6.5.1. Assessing the ability of the 2D Fisher-KPP equation to model cell-sheet wound closure

Participants: Abderrahmane Habbal, Hélène Barelli [Univ. Nice Sophia Antipolis, CNRS, IPMC], Grégoire Malandain [Inria, EPI Morpheme].

We address in this joint collaboration the ability of the widely used Fisher-KPP equations to render some of the dynamical features of epithelial cell-sheets during wound closure.

Our approach is based on nonlinear parameter identification, in a two-dimensional setting, and using advanced 2D image processing of the video acquired sequences. As original contribution, we lead a detailed study of the profiles of the classically used cost functions, and we address the "wound constant speed" assumption, showing that it should be handled with care.

We study five MDCK cell monolayer assays in a reference, activated and inhibited migration conditions. Modulo the inherent variability of biological assays, we show that in the assay where migration is not exogeneously activated or inhibited, the wound velocity is constant. The Fisher-KPP equation is able to accurately predict, until the final closure of the wound, the evolution of the wound area, the mean velocity of the cell front, and the time at which the closure occurred. We also show that for activated as well as for inhibited migration assays, many of the cell-sheet dynamics cannot be well captured by the Fisher-KPP model. Original unexplored utilizations of the model such as wound assays classification based on the calibrated diffusion and proliferation rate parameters is ongoing.[49] [76]



(a) (b) (c)

(d) (e) (f)

Figure 5. ***A regular wound assay*** *(a) Time evolution of wound area (in pixel). (b) Time evolution of the leading-edge length (in pixel). (c) 3D XT view at first and mid-rows. (d) Mean (in time) velocity of pixels located at the leading edge (in pixel/min). (e) Averaged (in space) leading-edge velocity (in pixel/min). (f) 2D XT view at first and mid-rows.*

(a) (b) (c)

Figure 6. ***A regular wound assay. Computational vs experimental wound evolution.*** *(a) Time variation of experimental (blue) versus computed (red) wound area (in pixel). (b) Time variation of the experimental (blue-dot) versus computed (red) migration rate (in pixel/min). (c) 3D XT view at first and mid-rows.*

(a) (b) (c)

Figure 7. ***An accelerating activated wound assay. Computational vs experimental wound evolution.*** *(a) Time variation of experimental (blue) versus computed (red) wound area (in pixel). (b) Time variation of the experimental (blue-dot) versus computed (red) migration rate (in pixel/min). (c) 3D XT view at first and mid-rows.*

POEMS Project-Team

6. New Results

6.1. Time domain wave propagation problems

6.1.1. Numerical methods in electromagnetism

Participant: Gary Cohen.

In the framework of contract GREAT, we implemented and compared two discontinuous Galerkin methods to solve Maxwell's equations for time dependent problems, the first using tetrahedral meshes (first used by Hesthaven), the second using hexahedral meshes with mass lumping. This comparison showed the undeniable superiority of the second method, 4-7 times faster (for orders from 2 to 4) for the same accuracy.

The ultimate goal of this program was the hybridization of those two types of meshes because the construction of purely hexahedral mesh for complex geometries is often difficult or almost impossible. A first approach was studied in the thesis Morgane Bergot, where the transition between the two grids was performed by the use of pyramids. The implementation of such elements is difficult and costly, we were interested in a transition mortars elements capable of hybridizing directly tetrahedra with flat faces and hexahedral with non-planar faces. This approach is promising and should lead to a rapid and efficient method. A theoretical study of the error and stability is conducted in collaboration with Eric Chung of CUHK (Chinese University of Hong Kong).

Moreover, always with E. Chung, we became interested in the construction of a discontinuous Galerkin method on hexahedral meshes offset for solving Maxwell's equations. This approach has two advantages : firstly, the shift naturally removes the spurious waves which appear with other approaches (which usually requires the introduction of a dissipative term to remove them). On the other hand, a phenomenon of super-convergence appears which should lead to a substantial time saving. A first study of the dispersion of this method led to a publication.

6.1.2. Solving the Homogeneous Isotropic Linear Elastodynamics Equations Using Potentials and Finite Elements.

Participants: Aliénor Burel, Patrick Joly.

The aim of this subject, investigated in collaboration with Marc Duruflé (Inria Bordeaux) and Sébastien Imperiale (Inria Saclay), is to use the classical theoretical decomposition of the elastodynamic displacement into two potentials referring to the pressure wave and the shear wave, and use it in a numerical framework. During the past two years, a method has been proposed for solving the Dirichlet problem (clamped boundary), successfully analysed and implemented, and for the free boundary conditions, we proposed an original method considering these boundary conditions as a perturbation of the Dirichlet conditions. This approach performs successfully in the time-harmonic regime but appears to give rise to severe instabilities in the time-dependent case after space and time discretization. Our investigations seem to prove that this instability is already present in the semi-discrete problem in space, but we are still looking for an explanation of this phenomenon.

6.1.3. Limiting amplitude principle in a two-layered medium composed of a dielectric and a metamaterial

Participants: Maxence Cassier, Christophe Hazard, Patrick Joly, Valentin Vinoles.

We are investigating this problem from both theoretical and numerical points of view. This is also the object of a collaboration with B. Gralak from the Institut Fresnel in Marseille.

This work is the time-domain counterpart of the research done at Poems about frequency domain analysis of metamaterials in electromagnetism, in the framework of the ANR Project METAMATH. One fundamental question is the link between the evolution / time harmonic problems via the limiting amplitude principle, in particular in the cases where the time harmonic problem fails to be well posed. This occurs, at certain frequencies, when one considers a transmission problem between a standard dielectric material and a dispersive material obeying for instance to the Drude model (other models as Lorentz materials or their generalization also give rise to the same results). Indeed, for well-chosen coefficients (which we refer as the critical case), there exist critical frequencies (only one frequency ω_c for the Drude model) for which the metamaterial behaves as a material whose equivalent electric permittivity and magnetic permeability are negative and precisely opposite to the ones of the dielectric medium : in such a situation, in the case of a plane interface, it is known that the time harmonic transmission problem is strongly ill-posed.

We have considered the evolution problem in a two-layered medium, when we consider a source term $f(x)\, e^{i\,\omega t}$ with frequency $\omega > 0$. In the non critical case, the limiting amplitude principle holds : for large times, the solution $u(x,t)$ of the evolution problem "converges" to a time harmonic solution of the form $u^\infty(x)\, e^{i\,\omega t}$. In the critical case, the limiting amplitude principle no longer holds. If $\omega \neq \omega_c$, the solution of the evolution problem behaves when $t \to +\infty$ to a "double frequency" solution of the form

$$u^\infty(x)\, e^{i\,\omega t} + u^\infty_{c,+}(x)\, e^{i\,\omega_c t} + u^\infty_{c,-}(x)\, e^{-i\,\omega_c t}.$$

If $\omega = \omega_c$, the solution blows up linearly at infinity :

$$u(x,t) \sim t\; u^\infty_c(x)\, e^{i\,\omega_c t} \quad (t \to +\infty)$$

where the function $u^\infty_c(x)$ is "concentrated" near the interface : this can be interpreted as an "interface resonance" phenomenon. We have performed various numerical experiments (using in particular the stabilized PMLs evoked in section 6.3.2) that illustrate this resonance phenomenon (cf figure 1).

Figure 1. Left : the interface wave. Right : solution at one point as a function of time.

From the mathematical point of view, the method we have used consists in rewriting the original problem as an abstract Schrödinger equation

$$i\,\frac{du}{dt} + Au = F\; e^{i\,\omega t}$$

where A is a self-adjoint operator in an appropriate Hilbert space H. The key of the analysis is the spectral theory of the operator A. This permits a quasi-explicit representation of the solution via the (generalized) diagonalization of A. This is achieved by combining a partial Fourier transform along the interface with Sturm-Liouville type techniques in the orthogonal direction. In the critical case, the resonance phenomenon appears to be linked to the fact that A admits a (single) eigenvalue of infinite multiplicity.

6.1.4. Finite differences method for nonlinear acoustic waves with fractional derivatives

Participant: Jean-François Mercier.

This subject is developed in collaboration with Bruno Lombard from LMA.

We develop a numerical method to study the wave propagation in a 1-D guide with an array of Helmholtz resonators, considering large amplitude waves and viscous boundary layers. The model consists in two coupled equations: a nonlinear PDE for the velocity in the tube (Burgers like equation) and a linear ODE describing the pressure oscillations in the Helmholtz resonators. The dissipative and dispersive effects in the tube and in the necks of the resonators are modelled by fractional derivatives expressed as convolution products with singular kernels. Based on a diffusive representation, the convolution kernels of the fractional derivatives are replaced by a finite number of memory variables that satisfy local ordinary differential equations. The procedure to compute weights and nodes of the diffusive representation of fractional derivatives is optimized. Moreover an adequate coupling between the PDE and the ODE is introduced to be sure that the discrete energy is decreasing. A splitting strategy is then applied to the evolution equations to obtain a stable scheme under the optimal CFL condition: the propagative part is solved by a standard TVD scheme for hyperbolic equations, whereas the diffusive part is solved exactly. This approach is validated by comparisons with exact solutions. The properties of the full nonlinear solutions are investigated numerically. In particular, the existence of acoustic solitary waves, due to the competition between dispersion and nonlinear effects, is confirmed.

6.2. Time-harmonic diffraction problems

6.2.1. Numerical computation of variational integral equation methods

Participants: Marc Lenoir, Nicolas Salles.

The discretization of 3-D scattering problems by variational boundary element methods leads to the evaluation of such elementary integrals as

$$\int_{S\times T} G\,(x,y)\;v\,(x)\,w\,(y)\;dx\,dy \text{ and } \int_{S\times T} \frac{\partial}{\partial n_y} G\,(x,y)\;v\,(x)\,w\,(y)\;dx\,dy \tag{6}$$

where v and w are polynomial basis functions, G is the Green kernel and S and T two planar polygons from the discretization of the boundary. Due to the singularity of the kernel, the numerical evaluation of these integrals may lead to inaccurate results when S and T are close to each other. We split G and its gradient into a regular part which involves classical numerical techniques and a singular part subject to our method. This new method consists in integrating exactly integrals such as

$$I = \int_{S\times T} v(x)\frac{1}{\|x-y\|}w(y)\,dx\,dy \text{ and } J_\zeta = \int_{S\times T} \frac{x-y}{\|x-y\|^{1+\zeta}}\,dx\,dy,\ \zeta\in\{0,2\}. \tag{7}$$

or numerically integrals such as:

$$\mathcal{L} = \int_{S\times T} v(x)\frac{e^{ik\|x-y\|}}{\|x-y\|}w(y)\,dx\,dy \tag{8}$$

where v and w are basis functions of order 0 or 1. The general approach relies on two steps.

Basic formulas : let $f\,(x,d)\ :\Omega\subset\mathbb{R}^n\times\mathbb{R}\longrightarrow\mathbb{R}$ a positively homogeneous function of degree q. By Euler's formula and Green's theorem we have the function $I(d)$ satisfies :

$$(q+n)\,I\,(d) = dI'\,(d) + \int_{\partial\Omega}(\overrightarrow{z}\,|\overrightarrow{\nu}\,)\,f\,(z,d)\,d\gamma_z, \quad \text{with } I\,(d) = \int_{\Omega} f\,(z,d)\,dz \tag{9}$$

where $\overrightarrow{\nu}$ is the exterior normal to Ω. Provided $d^{-(q+n)}\int_{\Omega} f\,(z,d)\,dz \to 0$ as $d\to+\infty$ one obtains

$$I\,(d) = d^{q+n}\int_{\partial\Omega}(\overrightarrow{z}\,|\overrightarrow{\nu}\,)\int_d^{+\infty}\frac{f\,(z,t)}{t^{q+n+1}}dt\,d\gamma_z. \tag{10}$$

When $f\,(z,d)$ does not depend on d and $q+n\neq 0$ then

$$I = \frac{1}{q+n}\int_{\partial\Omega}(\overrightarrow{z}\,|\overrightarrow{\nu}\,)\,f\,(z)\,d\gamma_z. \tag{11}$$

As long as the inner integral in (5) can be explicitly evaluated, both formulas reduce an n-dimensional integral to an $(n-1)$ one. When Ω is an n-dimensional polyhedron (such as $S\times T$ with $n=4$), $(\overrightarrow{z}\,|\overrightarrow{\nu}\,)$ is constant on each $(n-1)$-face of Ω, a simplification of crucial importance in the sequel.

The reduction process : we have obtained formulas for three types of geometrical configurations: S and T are (i) coplanar, (ii) in secant planes and (iii) in parallel planes. All these cases are treated using formulas (6) or (5) or both, depending on the relative positions of S and T. As an example, we present the simple but significant result for the self-influence coefficient ($S=T$). Let A_i be a vertex of the triangle, α_i the opposite side, B_i the orthogonal projection of A_i on α_i and $\gamma_i = \|A_iB_i\|$. After 3 successive reductions using formula (6), one obtains

$$I = \int_{S\times S}\frac{1}{\|x-y\|}dxdy = \frac{2\,|S|}{3}\sum_{i=1,3}\gamma_i R\,(A_i,\alpha_i)\,, \tag{12}$$

where $R(A_i,\alpha_i)$ is given analytically by ((i,jk) being a circular permutation of $(1,2,3)$)

$$R\,(A_i,\alpha_i) = \int_{\alpha_i}\frac{1}{\|A_i-y\|}dy = \operatorname{arg\,sinh}\frac{\|B_iA_k\|}{\gamma_i} - \operatorname{arg\,sinh}\frac{\|B_iA_j\|}{\gamma_i}. \tag{13}$$

Results for the 3-D Helmholtz equation with piecewise constant density have been obtained for all pairs of panels. Integral $\mathcal{L}$ (see formula (3)) can be reduced to a linear combination of 1-D or 2-D integrals when triangles have at least one common vertex; the resulting integrals have to be evaluated numerically but the final integrands are simple and regular on the domain of integration. For example, when $T=S$ and with piecewise constant basis functions, one has:

$$\mathcal{L} = \int_{S\times S}\frac{e^{ik\|x-y\|}}{\|x-y\|}\,dx\,dy = 4|S|\sum_{i=1}^{3}\gamma_i\int_{\alpha_i} f\,(\|A_i-y\|)\,ds_y \tag{14}$$

where $f(r) = i\dfrac{e^{ikr}-1-ikr+k^2r^2/2}{k^3r^4}$.

The extension to linear basis functions is in progress. Our method works also for 3-D Maxwell's equations with linear edge basis functions (for MFIE and EFIE). Despite some (possibly) lengthy calculations, the principle is rather straightforward and the method is quite flexible, leading to the reduction of 4-D integrals to a linear combination 1-D regular integrals which can be numerically or even explicitly evaluated. It is possible to use our method for Collocation technique, 2-D BEM and volume integral equations. A high degree of accuracy can be obtained, even in the case of nearly singular integrals. We will present the method and some results for 3-D Helmholtz equation.

6.2.2. Integral equations for modelling eddy current non destructive testing experiments

Participants: Marc Bonnet, Audrey Vigneron.

This work in collaboration with E. Demaldent (CEA LIST) is concerned with developing boundary element solvers for modelling eddy current non destructive testing experiments, taking into account the probe, the probed part and the surrounding air. Attention is focused in implementing Galerkin-type formulations, overcoming ill-conditioning arising in configurations involving high contrasts, and fast solvers. Among several possible integral formulations based on either Maxwell's equations or the eddy-current model, a weighted coupled formulation using a loop-tree decomposition of the trial and test spaces was found to perform adequately over the whole range of values of physical parameters typical of eddy-current NDT experiments.

6.2.3. Elastodynamic fast multipole method for semi-infinite domains.

Participants: Marc Bonnet, Stéphanie Chaillat.

The use of the elastodynamic half-space Green's tensor in the FM-BEM is a very promising avenue for enhancing the computational performances of 3D BEM applied to analyses arising from e.g. soil-structure interaction or seismology. This work is concerned with a formulation and computation algorithm for the elastodynamic Green's tensor for the traction-free half-space allowing its use within a Fast Multipole Boundary Element Method (FM-BEM). Due to the implicit satisfaction of the traction-free boundary condition achieved by the Green's tensor, discretization of (parts of) the free surface is no longer required. Unlike the full-space fundamental solution, the elastodynamic half-space Green's tensor cannot be expressed in terms of usual kernels such as $e^{ikr/r}$ or $1/r$. Its multipole expansion thus cannot be deduced from known expansions, and is formulated in this work using a spatial two-dimensional Fourier transform approach. The latter achieves the separation of variables which is required by the FMM. To address the critical need of an efficient quadrature for the 2D Fourier integral, whose singular and oscillatory character precludes using usual (e.g. Gaussian) rules, generalized Gaussian quadrature rules have been used instead. The latter were generated by tailoring for the present needs the methodology of Rokhlin's group. Extensive numerical tests have been conducted to demonstrate the accuracy and numerical efficiency of the proposed FMM. In particular, a complexity significantly lower than that of the non-multipole version was shown to be achieved. A full FM-BEM based on the proposed acceleration method for the half-space Green's tensor is currently under way. This treatment of the Green's tensor will be extended to other cases, e.g. layered semi-infinite media.

6.2.4. Domain decomposition methods for time harmonic wave propagation

Participants: Patrick Joly, Mathieu Lecouvez.

This work is motivated by a collaboration with the CEA-CESTA (B. Stupfel) through the PhD thesis of M. Lecouvez and is the object of a collaboration with F. Collino, co-advisor of the thesis with P. Joly.

We have considered first the case of the scalar Helmholtz equation for which we have developed a non overlapping iterative domain decomposition method based on the use of Robin type transmission conditions, in the spirit of previous works in the 90's by Collino, Després, and Joly.

The novelty of our approach consists in using new transmission conditions using some specific impedance operators in order to improve the convergence properties of the method (with respect to more standard Robin conditions). Provided that such operators have appropriate functional analytic properties, the theory shows that one achieves geometric convergence (in opposition the the slow algebraic convergence obtained with standard methods). These properties prevent the use of local impedance operator, a choice that was commonly done for the quest of optimized transmission conditions (following for instance the works of Gander, Japhet, Nataf). We propose a solution that uses nonlocal integral operators using appropriate Riesz potentials, the important feature of which being their singularity at the origin. To overcome the disadvantage of dealing with completely nonlocal operators, we suggest to work with truncated kernels, involving adequate smooth cut-off function. The results we have obtained are

- A complete theoretical justification of the exponential convergence of the algorithm in the 2D case for smooth enough interfaces. The extension to 3D is in progress : the case of a spherical interface is in particular completely understood.
- An heuristic analysis of the influence of the truncation procedure (several choices are possible) on the convergence of the method, together with a (semi-analytical) search for optimal values of the parameters involved in the method to improve the convergence rate.
- The implementation of the method in 2D and an intensive campaign of numerical validation of the method that appear to provide very good performance and seem to indicate that the method is quite robust with respect to increasing frequency (which remains to be proven). Let us however mention that, not so important but unexpected phenomena, due to space discretization, have been observed and remain to be explained. The implementation in 3D, in cooperation with M. Duruflé, is in progress.

The relevant application at CESTA being electromagnetism, the extension of the method to 3D Maxwell's equations, which proposes new non trivial difficulties, has been initiated.

As the development and the theoretical understanding of these new domain decomposition methods clearly exceed the content of one single thesis, we have proposed an ANR project on this topic, in collaboration with X. Claeys (Paris VI).

6.2.5. Time harmonic aeroacoustics

Participant: Jean-François Mercier.

This subject is treated in collaboration with Florence Millot (Cerfacs). We are still working on the numerical simulation of the acoustic radiation and scattering in presence of a mean flow. Up to now we have considered Galbrun's equation, but for 3D configurations it requires to introduce many unknowns. Therefore we focus now on the alternative model of Goldstein's equations. When the fluid flow and the source are potential, the acoustic perturbations are also potential and the velocity potential φ satisfy a simple scalar model. For a general flow, this model is slightly modified and is called Goldstein's equations. A new vectorial unknown ξ is introduced, satisfying a transport equation coupled to the velocity potential. φ satisfies the same modified Helmholtz's equation than in the potential flow case, in which ξ plays the role of a source term. The advantage of Goldstein's formulation compared to Galbrun's model is that the vectorial unknown vanishes in the areas where the flow is potential.

For a general flow ξ can be expressed versus φ as a convolution formula along the flow streamlines. The situation is much simpler for slow flows since the convolution formula can be simplified and the link between ξ and φ becomes explicit. Then Goldstein's equations can be solved by using continuous finite element (discontinuous elements must be used in the general case). We have proved theoretically that when replacing the general convolution formula by the "slow flow" approximation, the error on the velocity potential is small, bounded by the square of the flow velocity. This has been done for a simpler case, a shear flow, for which the streamlines are just parallel lines. Numerical tests have confirmed the square law for the error.

6.2.6. Mathematical and numerical analysis of metamaterials

Participants: Patrick Joly, Anne-Sophie Bonnet-Ben Dhia, Patrick Ciarlet, Sonia Fliss, Camille Carvalho, Valentin Vinoles, Christian Stohrer.

Metamaterials are artificial composite materials having the extraordinary electromagnetic property of negative permittivity and permeability at some frequencies . Both of sign-changing coefficients and high contrast homogenization raise new mathematical and numerical challenges. The ANR METAMATH is devoted to the study of those problems. We perform analysis both in time domain (see sections 6.1.3 and 6.3.2) and harmonic domain.

6.2.6.1. Time-harmonic transmission problems involving metamaterials

A special interest is devoted to the transmission of an electromagnetic wave between two media with opposite sign dielectric and/or magnetic constants. As a matter of fact, applied mathematicians have to address challenging issues, both from the theoretical and the discretization points of view. In particular, it can happen that the problem is not well-posed in the classical frameworks (H^1 for the scalar case, $H(curl)$ for the vector case). During 2013, we addressed the issues below.

The numerical analysis of the well-posed scalar eigenproblem discretized with a classical, H^1 conforming, finite element method, for arbitrarily shaped interfaces can be carried out with the help of T-coercivity. This work complements the paper Chesnel-Ciarlet, published in Numerische Mathematik, which handled simpler interface configurations (see also §6.2.6.2).

As a second topic, we investigated the case of a scattering problem with a 2D corner interface which can be ill-posed (in the classical H^1 framework). When this is the case, the part of the solution which does not belong to H^1 can be described as a wave which takes an infinite time to reach the corner: this "black-hole" phenomenon is observed in other situations (elastic wedges for example). We have proposed a numerical approach to approximate the solution which consists in adding some Perfectly Matched Layers in the neighbourhood of the corner. As an alternate choice, a T-coercivity approach is also being currently developed to solve the discrete problem.

Last, we studied the transmission problem in a purely 3D electromagnetic setting from a theoretical point of view. We proved that the Maxwell problem is well-posed if and only if the two associated scalar problems (with Dirichlet and Neumann boundary conditions) are well-posed. Numerical analysis of the discretized models (edge elements) is under way.

L. Chesnel left our project in March 2013 after he completed his PhD thesis on these topics. He is currently a post-doc fellow at Aalto University (Finland).

6.2.6.2. Modeling of plasmonic devices

Plasmonic surface waves occur at the interface between the vacuum (or a dielectric) and a metal, at optical frequencies, when the dielectric permittivity ε of the metal has a small imaginary part and a large negative real part. Neglecting the dissipation effects, we have to study electromagnetic problems with a sign-changing ε. An in-depth analysis has been done by Lucas Chesnel during his PhD. In the context of the PhD of Camille Carvalho, we extended the results obtained previously by Lucas Chesnel to more realistic configurations. First, we studied the diffraction of a transversely polarized plane wave by a cylindrical metallic inclusion, when the section of the inclusion presents edges (cf. §6.2.6.1). Then, we considered a related spectral problem in view of studying plasmonic guided waves. The spectral theory is far from obvious. In particular, we have to introduce a non-selfadjoint formulation which provides physical real eigenvalues and complex spurious ones. For both the diffraction problem and the spectral problem, a MATLAB code has been developed, where Perfectly Matched Layers are introduced at the corners to take into account the presence of black-hole waves seemingly absorbed by the corners. The convergence of the finite element discretization (including convergence of the eigenvalues) has been proved (see §6.2.6.1).

6.2.6.3. Study of metamaterials via numerical homogenization

Recently, we have started to study the numerical approximation of the full models, using the HMM (Heterogeneous Multiscale Method). Recall that the full model is obtained via periodization of a local model that includes slow and fast variations. With this HMM approach, computations are carried out on a global mesh, whereas the action of the test-functions is computed at a local level to take into account the fast variations. As a first step, we have begun by the application of HMM for the time-harmonic scalar problem. The case of uniformly bounded coefficients has been addressed. The more general case of non-uniformly bounded coefficients, also called the high-contrast case, is now under scrutiny. It is hoped that one can recover some extra-ordinary properties of the metamaterials with this latter case.
C. Stohrer arrived as a post-doc fellow this fall.

6.3. Absorbing boundary conditions and absorbing layers

6.3.1. New transparent boundary conditions for time harmonic acoustic and elastic problems in anisotropic media

Participants: Anne-Sophie Bonnet-Ben Dhia, Antoine Tonnoir, Sonia Fliss.

This topic is developed in collaboration with Vahan Baronian (CEA). Non destructive testing (NDT) is a common method to check the quality of structures and is widely used in industrial applications. Typically, in aircraft design, it is required to control structures like plates. Efficient and accurate numerical methods are required to simulate NDT experiments.

In our case, we want to study the diffraction of a time harmonic wave by a bounded defect in an infinite anisotropic elastic plate. The difficulty is to find a way to restrict the finite element computation to a small box containing the defect. Indeed classical methods such as the perfectly matched layers fail when the medium is anisotropic.

Up to now we considered the simpler case of an infinite dissipative 2D medium.

Our idea, inspired by the work of Sonia Fliss and Patrick Joly for periodic media, is to consider five domains recovering the whole plane:

- a square that surrounds the defect in which we have a finite element representation of the solution,
- and four half-spaces parallel to the four edges of the square, in which we can give an analytical representation of the solution thanks to the Fourier transform.

The different unknowns are coupled by well-chosen transmission relations which ensure the compatibility between the five representations.

The method has been validated successfully in the case of anisotropic acoustic media and the implementation for the case of elasticity is in progress. The mathematical properties of the formulation and the efficiency of the method strongly depend on the presence or not of overlaps between the finite element box and the four half-planes. The formulation with overlaps has good Fredholm properties but the well-posedness for all frequencies is proved only for the formulation without overlaps.

6.3.2. Perfectly Matched Layers in negative index metamaterials

Participants: Patrick Joly, Eliane Bécache, Valentin Vinoles.

The simulation of waves in unbounded domains requires methods to artificially truncate the computational domain. One of the most popular ones to do so is the Perfectly Matched Layers (PMLs) which are effective and stable for non dispersive isotropic media. For non dispersive anisotropic media, we established a necessary stability condition in 2004 : PMLs are unstable in presence of so called-backward waves.

We are interested here in dispersive media and more specifically in Negative Index Metamaterials (NIMs), also called left-handed media. Those media have negative permittivity and permeability at some frequencies due to microscopic resonating structures. Since the 1990s, NIMs are the subject of active researches due to their promising applications : superlens, cloaking, improved antenna, etc.

In a first step, we consider a simple model of NIMs : the Drude model. For this model, a plane wave analysis shows the simultaneous presence of both forward and backward waves and numerical simulations confirm the instability of standard PMLs (cf figure 2) that result from complex changes of variable leading to the following modification of the spatial derivatives

$$\partial_x \longrightarrow \left(1+\frac{\sigma_x(x)}{i\omega}\right)^{-1}\partial_x \quad \text{and} \quad \partial_y \longrightarrow \left(1+\frac{\sigma_y(y)}{i\omega}\right)^{-1}\partial_y$$

where $\sigma_x(x) > 0$ and $\sigma_y(y) > 0$ are the damping terms. Inspired by works of the physics community, we propose more general changes of variable

$$\partial_x \longrightarrow \left(1+\frac{\sigma_x(x)}{i\omega\psi(\omega)}\right)^{-1}\partial_x \quad \text{and} \quad \partial_y \longrightarrow \left(1+\frac{\sigma_y(y)}{i\omega\psi(\omega)}\right)^{-1}\partial_y$$

where $\psi(\omega)$ is a function to be chosen judiciously. We have generalised the previous necessary stability condition for those new PMLs, called Stabilized Perfectly Matched Layers, for dispersive media. This analysis allows us to understand the instabilities observed for standard PMLs in NIMs and to propose a choice of functions $\psi(\omega)$ which take into account the backward waves and stabilize the PMLs as confirmed by numerical simulations (cf figure 2).

Figure 2. Left : the standard PMLs are unstable. Right : the Stabilized PMLs are stable.

6.3.3. Perfectly Matched Layers in plasmas

Participants: Patrick Joly, Eliane Bécache, Valentin Vinoles.

This work was done during the internship of Guillaume Chicaud in the framework of the ANR CHROME which concerns the study of electromagnetic wave propagation in plasmas. Our aim is to develop efficient and robust codes to simulate wave propagation in unbounded plasmas models. The simulation of waves in plasmas requires technics to bound the computational domain. As plasmas are dispersive media where backward waves may occur, the difficulties to construct stable PMLs are analogous to the ones encountered for Negative Index Metamaterials (cf 6.3.2). This work is a preliminary study of this topics, in a simplified model, the case of a 2D anisotropic uniaxial plasma. It consists first in analyzing the presence of backward waves with a plane wave analysis. The second step was to implement the equations using standard PMLs and to confirm the expected

instabilities. Finally, we proposed stabilized PMLs (SPMLs), inspired by the work done in metamaterials (see section 6.3.2).

The continuation of this project will constitute the subject of the post-doc of Maryna Kachanovska.

6.4. Waveguides, resonances, and scattering theory

6.4.1. An improved modal method in non uniform acoustic waveguides

Participant: Jean-François Mercier.

This topic is developed in collaboration with Agnès Maurel (Langevin Institute ESPCI).
We develop modal methods to study the scattering of an acoustic wave in a non uniform waveguide. Usual modal approaches are efficient only when a rather large number of evanescent modes are taken into account. An improved representation has been proposed in which an additional transverse mode and an additional unknown modal component are introduced. This so called boundary mode helps to better satisfy the Neumann boundary conditions at the varying walls. A system of coupled ordinary differential equations is obtained and is found to remain coupled in the straight part of the waveguide which implies that the classical radiation condition cannot be applied directly at the inlet/outlet of the scattering region.

We revisit the coupled mode equations in order to derive an improved system, in which the additional mode can be identified as evanescent mode, and then adapted to define radiation conditions. This makes possible the implementation of efficient numerical multimodal methods (like the admittance matrix method) and also approximate solutions can be found using the Born approximation. The numerical tests have shown that our method is very efficient to reduce the number of degree of freedom: adding to the boundary mode, it is sufficient to take only the propagative modes to get very good results. This is in particular interesting at low frequency when only the plane mode propagates. In the low frequency regime, the system can be solved analytically, using the Born approximation, leading to improved approximate equations compared to the usual Webster's approximation.

6.4.2. Construction of non scattering perturbations in a waveguide

Participants: Anne-Sophie Bonnet-Ben Dhia, Eric Lunéville.

This work is done in collaboration with Sergei Nazarov from Saint-Petersbourg University and during the internship of Yves Mbeutcha. We consider a two-dimensional homogeneous acoustic waveguide and we aim at designing deformations of the boundary which are invisible at a given frequency (or more generally at a finite number of given frequencies) in the sense that they are non scattering. To find such invisible perturbations, we take advantage of the fact that there are only a finite number of propagative modes at a given frequency in a waveguide. As a consequence, the invisibility is achieved by canceling a finite number of scattering coefficients, and an invisible deformation only produces an exponentially decreasing scattered field, not measurable in the far field.

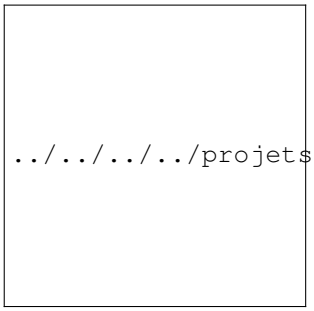
The first step consists in studying the effect of a small deformation, of amplitude ε. The asymptotic analysis allows to derive the first order terms of the scattering coefficients, as integrals involving the function describing the deformation. This leads to express the deformation as a linear combination of some explicit (compactly supported) functions, so that invisibility is satisfied if and only if the coefficients of the linear combination are solution of a fixed point equation. The key point is that we can prove, using the results of the asymptotic analysis, that the function of this fixed point equation is a contraction for ε small enough. This proves the existence of invisible deformations of amplitude ε. Moreover, it provides a natural algorithm to compute the invisible deformation.

This has been tested numerically and the results are in perfect agreement with the theory. At low frequency, the good news is that ε can be taken quite large (the amplitude of the deformation may be half the size of the guide). But this deteriorates when the frequency increases.

6.4.3. Localized modes in unbounded perturbed periodic media

Participants: Patrick Joly, Sonia Fliss, Elizaveta Vasilevskaya.

This topic is investigated in collaboration with Bérangère Delourme (Univ. Paris XIII) and constitutes the subject of the E. Vasilevskaya's PhD thesis. We are interested in a 2D propagation medium which is a localized perturbation of a reference homogeneous periodic reference medium. This reference medium is a "thick graph", namely a thin structure (the thinness being characterized by the parameter $\delta > 0$) whose limit when δ tends to 0 is a periodic graph. This is for instance the case of the thick periodic ladder and the thick periodic rectangular grid of figure. The perturbation consists in changing only the geometry (and not the material properties) of the reference medium by modifying the thickness of one of the lines of the reference medium as illustrated by figure with the perturbed ladder and perturbed grid (see figure 3). The question we investigate is whether such a geometrical perturbation is able to produce localized eigenmodes (for the ladder) or guided modes (for the grid). We have investigated this question when the propagation model is the scalar Helmholtz equation with Neumann boundary conditions (in opposition to Dirichlet conditions that have been more studied in the literature - see the works by S. Nazarov for instance). This amounts to solving an eigenvalue problem for the Laplace operator in an unbounded domain : the associated self-adjoint operator has a continuous spectrum with a band gap structure and the eigenvalues are searched in the gaps.



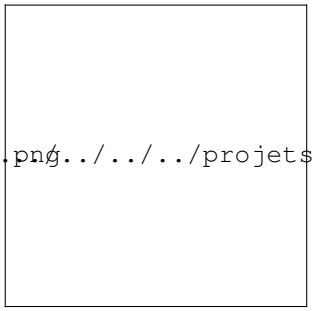


Figure 3. Left : periodic ladder (non perturbed/perturbed). Right : periodic "thick graph" (non perturbed/perturbed). The propagation domain is in grey.

With Neumann boundary conditions, we can use for the theoretical study an asymptotic analysis with respect to δ: indeed, it is well known (see in particular the works by Exner, Kuchment, Post) the limit model when δ tends to 0, is the Helmholtz equation on the graph : 1D Helmholtz equations on each branch completed by continuity and Kirchoff transmission conditions at each node. The geometrical perturbation of the original medium results into a perturbation of the Kirchoff conditions on the nodes of the modified line. The spectral analysis of the limit problem can be done completely by hand and the existence of eigenmodes for the thick medium is ensured, for δ small enough, by the existence of corresponding eigenmodes for a limit "1D operator" whose spectrum appears to possess an infinity of band gaps in each of which eigenvalues can exist, due to the perturbation. Following this idea, we have been able to prove the existence of localized modes in the case of the ladder provided that the geometrical perturbation consists in diminishing the width of one rung. One can even prove that one can produce more and more localized modes, corresponding to larger and larger frequencies, when δ is smaller and smaller. On the contrary, we conjecture that there is no localized modes when we enlarge the rung. The extension of these results to the existence of guided modes in the case of the grid in progress.

For the numerical computation of such localized modes, we have adapted the DtN approach discussed in the activity report of 2012. We gave in figure 4 an example of computed localized mode in the case of the ladder : this mode is geometrically confined at the neighbourhood of the modified rung.

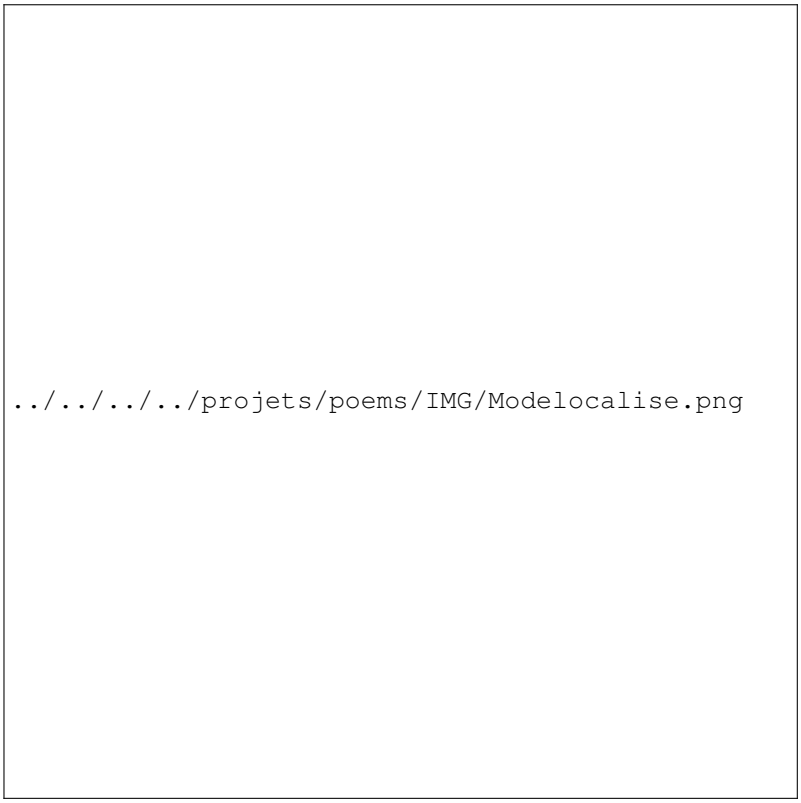


Figure 4. Localized mode in the perturbed ladder.

6.5. Asymptotic methods and approximate models

6.5.1. Homogenization and interfaces

Participants: Sonia Fliss, Valentin Vinoles.

This topic is developed in collaboration with Xavier Claeys (LJLL, Paris VI).

The mathematical modelling of electromagnetic metamaterials and the homogenization theory are intimately related because metamaterials are precisely constructed by a periodic assembly of small resonating micro-structures involving dielectric materials presenting a high contrast with respect to a reference medium. In the framework of the ANR Metamath (see 6.2.6), we wish to look carefully at the treatment of boundaries and interfaces that are generally poorly taken into account by the first order homogenization.

This question is already relevant for standard homogenization (ie without high contrast). Indeed, the presence of a boundary induces a loss of accuracy due to the inadequateness of the standard homogenization approach to take into account boundary layer effects. Our objective is to construct approximate effective boundary conditions that would restore the desired accuracy.

We first considered a plane interface between a homogeneous and the periodic media in the standard case without high-contrast. We obtained high order transmission conditions between the homogeneous media and the periodic media. The technique we used involves matched asymptotic expansions combined with standard homogenization ansatz. Those conditions are non standard : they involve Laplace-Beltrami operators at the interface and requires to solve cell problems in infinite periodic waveguides. The derivation of the corresponding error estimates is in progress. The analysis is based on a original combination of Floquet-Bloch and a periodic version of Kondratiev technique.

The next step will be to consider the same problem but with a high-contrast periodic media in collaboration with Guy Bouchitté, a french expert in high contrast homogenization.

6.5.2. Effective boundary conditions for thin periodic coatings

Participants: Mathieu Chamaillard, Patrick Joly.

This topic is the object of a collaboration with Houssem Haddar (CMAP École Polytechnique). We are interested in the construction of "equivalent" boundary condition for the diffraction of waves by an obstacle with smooth boundary Γ covered with a thin coating of width δ whose physical characteristics vary "periodically" along Γ with a period proportional to the small parameter δ. For a general boundary Γ, the notion of periodicity is ambiguous: we have chosen to define the coating as the image, or the deformation, by a smooth mapping ψ_Γ of a flat layer of width δ (the reference configuration) that preserves the normals, which appears consistent with a manufacturing process. The electromagnetic parameters in the coating are then defined as the images through ψ_Γ of periodic functions in the reference configuration.

We have first considered the case of the scalar wave equation when the homogeneous Neumann condition is applied on the boundary of the obstacle. Using an asymptotic analysis in δ, which combines homogenization and matched asymptotic expansions, we have been able to establish a second order boundary condition of the form

$$\partial_\nu u + (\delta B_\Gamma^1 + \delta^2 B_\Gamma^2)u = 0,$$

where B_Γ^1 and B_Γ^2 are second order tangential differential operators along Γ. The coefficients of these operators depend on both the geometrical characteristics of Γ (through the curvature tensor), the deformation mapping ψ_Γ and the material properties of the coating, through the resolution of particular unbounded cell problems in the flat reference configuration. When the coating is homogeneous, we have checked that one recovers the well known second order thin layer condition. We have moreover proven that this approximate condition provides in $\mathcal{O}(\delta^3)$.

6.5.3. Thin Layers in Isotropic Elastodynamics

Participants: Marc Bonnet, Aliénor Burel, Patrick Joly.

This research is concerned with the numerical modelling of non-destructive testing experiments using ultrasonic waves. Some materials, e.g. composite materials, involve thin layers of resin. The numerical modelling of such thin layers can be problematic as they result in very small spatial mesh sizes. To alleviate this difficulty, we develop an approach based on an asymptotic analysis with respect to the layer thickness ε, aiming to model the thin layer by approximate effective transmission conditions (ETCs), which remove the need to mesh the layer. So far, ETCs that are second-order accurate in ε have been formulated, justified, implemented and numerically validated, for 2-D and 3-D configurations involving planar interfaces of constant thickness. In particular, the continuous evolution problem is shown to be stable, and a time-stepping scheme that essentially preserves the stability requirement on the time step is proposed. Extension of this work to 2-D and 3-D configurations involving a curved layer is ongoing.

6.5.4. Mathematical modelling of electromagnetic wave propagation in electric networks.

Participants: Geoffrey Beck, Patrick Joly.

This topic is developed in collaboration with S. Imperiale (Inria Saclay) in the framework of the ANR project SODDA, in collaboration with CEA-LETI, about the non destructive testing of electric networks. This is the subject of the PhD thesis of G. Beck.

We investigate the question of the electromagnetic propagation in thin electric cables from a mathematical point of view via an asymptotic analysis with respect to the (small) transverse dimension of the cable: as it has been done in the past in mechanics for the beam theory from 3D elasticity, we use such an approach for deriving simplified effective 1D models from 3D Maxwell's equations.

During last year, we have achieved some progress in various directions:

- Single wire coaxial cables. This is the direct continuation of what has been done last year. Concerning the lowest order, the telegraphist's model, we have extended the error analysis, previously restricted to non lossy cylindrical cables to very general cases. Technically, this relies on time Laplace transform and new, parameter dependent, Poincaré-Friedrichs inequalities. From the numerical point of view, in collaboration with M. Duruflé, we have initiated a quantitative comparison between the full 3D model and our 1D model. Furthermore we have derived and studied a higher order generalized telegraphist's equation that include dispersive effects through nonlocal capacity and inductance operators. The corresponding mathematical analysis is in progress.
- Multiple wires cables. The objective here was to extend our approach to cables containing N conducting wires. Our results into a vectorial generalized telegraphist's model with $2N$ (2 for each wire) 1D unknowns, N electrical potentials and N currents. This model involves in particular a capacity matrix C, an inductance matrix L, a resistance matrix R and a conductance matrix G, whose properties have been deeply investigated, which allowed us to justify rigorously and extend some results from the electrical engineering literature. In the most general case, the effective models also involve time memory terms with matrix valued convolution kernels.
- Junction of cables. This is a new and essential step towards the modelling of networks. We have started the case of junctions of single wire cables via the method of matched asymptotic expansions in the spirit of the PhD thesis of A. Semin.

6.5.5. Elastic wave propagation in strongly heterogeneous media

Participants: Simon Marmorat, Patrick Joly.

This subject enters our long term collaboration with CEA-LIST on the development of numerical methods for time-domain non destructive testing experiments using ultra-sounds, and is realized in collaboration with Xavier Claeys (LJLL, Paris VI). We aim at developing an efficient numerical approach to simulate the propagation of waves in a medium made of many small heterogeneities, embedded in a smooth (or piecewise smooth) background medium, without any particular assumption (such as periodicity) on the spatial distribution of these heterogeneities. The figure 5 is a snapshot of a simulation inside such a medium, computed thanks to classical simulation tools: to reach satisfying accuracy, one has to use mesh refinement in the vicinity of the heterogeneities, which greatly increases the computational cost of the method.

Figure 5. Snapshot of a simulation in the medium of interest, using high-order finite element method as well as local mesh refinement and local time stepping around the heterogeneities.

By considering the medium with defects as a perturbation of the smooth one, we have derived an auxiliary model in the acoustic case, involving the defect-free wave operator and some volume Lagrange multipliers which account for the presence of the defects. These Lagrange multipliers are unknown functions defined on the defects and live in some infinite dimensional functional space. Exploiting the smallness of the defects, we have shown thanks to matched asymptotic analysis that the aforementioned functional space may be well described by a finite number N of profile functions: we propose an asymptotic model by looking for the Lagrange multipliers into the space spanned by these N profile functions, and we have shown that the error hence made is controlled by ε^N, ε being the characteristic size of the defects, assumed to be small.

On a computational point of view, the asymptotic model is much easier to solve than the original one since it can be discretized using a computation mesh that ignores the presence of the heterogeneities, the Lagrangian multipliers being computed by solving a linear system of size N. A resolution of this model has been implemented in the 1D and in the 2D case, and a rigorous error estimate has been established.

6.6. Imaging and inverse problems

6.6.1. Sampling methods in waveguides

Participants: Laurent Bourgeois, Sonia Fliss, Eric Lunéville, Anne-Claire Egloffe.

First, we have adapted the modal formulation of sampling methods (Linear Sampling Method and Factorization Method) to the case of a periodic waveguide in the acoustic case. This study is based on the analysis of the far field of scattering solutions in cylindrical waveguides, in particular for the fundamental solution, which enables us to obtain a far field formulation of sampling methods, and then a modal formulation of such methods. The aim of the inverse problem is to retrieve a defect (that is a loss of periodicity) from the scattered fields which correspond to the incident fields formed by the Floquet modes. Some convincing numerical experiments have shown the feasibility of the method. Secondly, going back to the homogeneous waveguide in the acoustic case, we have started a study of the sampling methods in a more realistic situation, that is the data (emission and reception) are measured on the boundary of the waveguide in the time domain. This was the subject of Anne-Claire Egloffe's post-doc. The aim is to use the modal formulation of the sampling methods at all frequencies and recompose the best possible image of the defect. Some first encouraging results have been obtained when the spectrum of the incident signal is centered at a rather low frequency (corresponding to 3 propagating guided modes).

6.6.2. Space-time focusing on unknown scatterers

Participants: Maxence Cassier, Patrick Joly, Christophe Hazard.

This topic concerns the studies about time-reversal in the context of Maxence Cassier's thesis. We are motivated by the following challenging question: in a propagative medium which contains several unknown scatterers, how can one generate a wave that focuses selectively on one scatterer not only in space, but also in time? In other words, we look for a wave that 'hits hard at the right spot'. Such focusing properties have been studied in the frequency domain in the context of the DORT method ("Decomposition of the Time Reversal Operator"). In short, an array of transducers first emits an incident wave which propagates in the medium. This wave interacts with the scatterers and the transducers measure the scattered field. The DORT method consists in doing a Singular Value Decomposition (SVD) of the scattering operator, that is, the operator which maps the input signals sent to the transducers to the measure of the scattered wave. It is now well understood that for small and distant enough scatterers, each singular vector associated with a non zero singular value generates a wave which focuses selectively on one scatterer. Can we take advantage of these spatial focusing properties in the frequency domain to find the input signals which generate a time-dependent wave which would be also focused in time? Since any frequency superposition of a family of singular vectors associated with a given scatterer leads to a spatial focusing, the main question is to synchronize them by a proper choice of their phases. The method we propose is based on a particular SVD of the scattering operator related to its symmetry. The signals we obtain do not require the knowledge of the locations of the scatterers. We compare it with some "optimal" signals which require this knowledge. Our study is illustrated by a two dimensional acoustic model where both scatterers and transducers are assumed pointlike (see figure 6).

6.6.3. The exterior approach to retrieve obstacles

Participant: Laurent Bourgeois.

This theme is a collaboration with Jérémi Dardé from IMT (Toulouse). The aim is to find a fixed Dirichlet obstacle in a bounded domain by using some redundant boundary conditions (Cauchy data) on the accessible part of the boundary, while the boundary conditions are unknown on the inaccessible part of the boundary. We wish to adapt the exterior approach developped for the Laplace equation and the Stokes system to the case of time evolution problems, in particular the heat equation. The exterior approach consists in defining a decreasing sequence of domains that converge in some sense to the obstacle. More precisely, such iterative approach is based on a combination of a quasi-reversibility method to update the solution of the ill-posed Cauchy problem outside the obstacle obtained at previous iteration and of a level set method to update the obstacle with the help of the solution obtained at previous iteration. We have already introduced two different mixed formulations of quasi-reversibility for the ill-posed heat equation with lateral Cauchy data in order to use standard Lagrange finite elements.

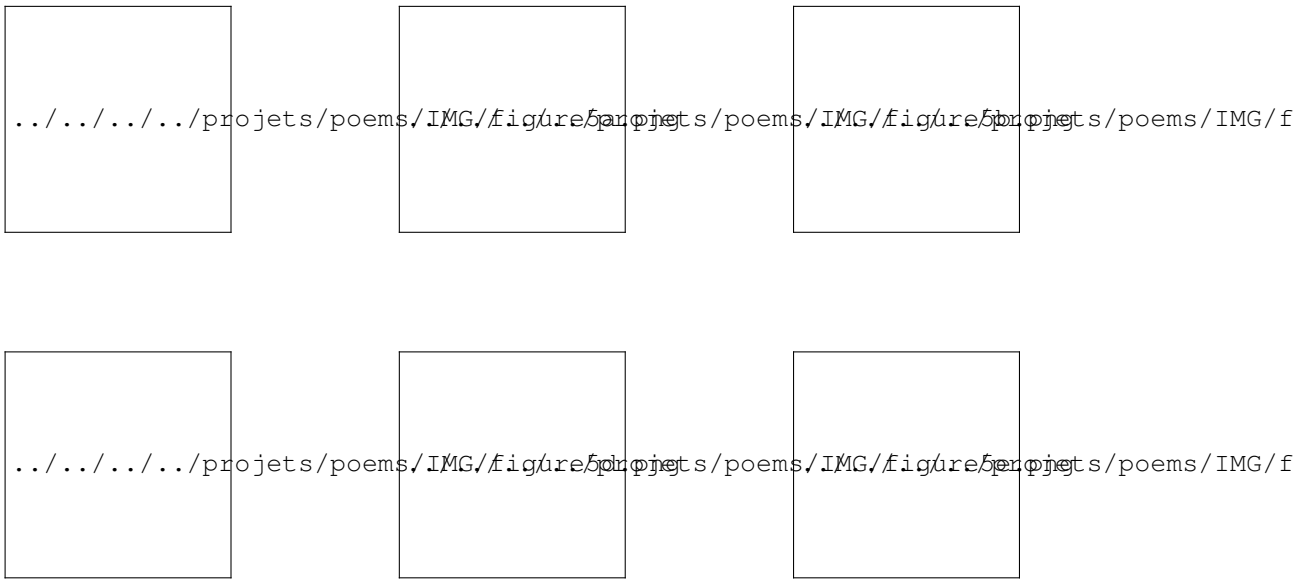


Figure 6. The case of a scattering reference medium perturbed by two obstacles (the white circles) : modulus of the field generated by 128 transducers (left edge of each figure) at different times.

6.6.4. Uniqueness and stability of inverse problems

Participant: Laurent Bourgeois.

In collaboration with Laurent Baratchart and Juliette Leblond from APICS (Nice), we have proved uniqueness for the inverse Robin problem with a boundary coefficient in L^∞ in the 2D case, for the Laplace equation in the divergence form. The result is based on complex analysis. We have also established an abstract Lipschitz stability result for inverse problems such that the set of parameters is a compact and convex subset of a finite dimensional space. In particular, such result can be applied to the previous inverse Robin problem.

6.6.5. Interior transmission problem

Participant: Anne-Sophie Bonnet-Ben Dhia.

This work is in collaboration with Lucas Chesnel (Aalto University, Finland). During this year, we investigated a two-dimensional interior transmission eigenvalue problem for an inclusion made of a composite material. This problem plays a central role in the theory of the corresponding inverse problem. We considered configurations where the difference between the parameters of the composite material and the ones of the background change sign on the boundary of the inclusion. In a first step, under some assumptions on the parameters, we extended the variational approach of the T-coercivity to prove that the transmission eigenvalues form at most a discrete set. In the process, we also provided localization results. Then, we study what happens when these assumptions are not satisfied. The main idea is that, due to very strong singularities that can occur at the boundary, the problem may lose Fredholmness in the natural H^1 framework. Using Kondratiev theory, we proposed a new functional framework where the Fredholm property is restored.

6.6.6. Flaw identification using elastodynamic topological derivative or transmission eigenvalues

Participants: Marc Bonnet, Rémi Cornaggia.

This work is in collaboration with C. Bellis (LMA, CNRS, Marseille), F. Cakoni (Univ. of Delaware, USA) and B. Guzina (Univ. of Minnesota, USA). The concept of topological derivative (TD) quantifies the perturbation induced to a given cost functional by the nucleation of an infinitesimal flaw in a reference defect-free body, and may serve as a flaw indicator function. In this work, the TD is derived for three-dimensional crack identification exploiting over-determined transient elastodynamic boundary data. This entails in particular the derivation of the relevant polarization tensor, here given for infinitesimal trial cracks in homogeneous or bi-material elastic bodies. Simple and efficient adjoint-state based formulations are used for computational efficiency, allowing to compute the TD field for arbitrarily shaped elastic solids. The latter is then used as an indicator function for the spatial location of the sought crack(s). The heuristic underpinning TD-based identification, which consists in deeming regions where the TD is most negative as the likeliest locations of actual flaws and on formulating higher-order topological expansions in the elastodynamic case, has (with C. Bellis and F. Cakoni) been given a partial justification within the limited framework of acoustic inverse scattering using far-field data. Current investigations (M. Bonnet, R. Cornaggia) include setting up and justifying the formulation of higher-order topological expansions for the elastostatic and elastodynamic cases.

Another ongoing research on a related topic addresses the use of transmission eigenvalues (TEs), i.e. values of the wave number for which the homogeneous interior transmission problem (ITP) related to the scattering scattering of time-harmonic elastic waves by aninhomogeneity D admits non-trivial solutions. This works (R. Cornaggia, in collaboration with C. Bellis, F. Cakoni, B. Guzina) aims on the one hand to understand better how to compute the TEs -if any- in the case where D's characteristics vary periodically. On the other hand it looks for how a previously obtained knowledge of the TE set could be the basis of an identification process. In a preliminary study considering 1-D elastic beams with periodically varying section over a length L, gradient elasticity was found to be a well-suited homogenization model to both compute the TEs and identify L, the periodic cell length and the damage parameter from available values of the TEs.

6.6.7. Topological derivative in anisotropic elasticity

Participant: Marc Bonnet.

This work is in collaboration with G. Delgado (PhD student, CMAP Ecole Polytechnique and EADS IW). Following up on previous work on the topological derivative (TD) of displacement-based cost functionals in anisotropic elasticity, a TD formula has been derived and justified for general cost functionals that involve strains (or displacement gradients) rather than displacements. The small-inclusion asymptotics of such cost functionals are quite different than in the previous case, due to the fact that the strain perturbation inside an elastic inclusion has a finite, nonzero asymptotic value in the limit of a vanishingly small inclusion. Cost functionals of practical interest having this format include von Mises equivalent stress (often used in plasticity or failure criteria) and energy-norm error functionals for coefficient-identification inverse problems. This TD formulation has been tested on 2D and 3D numerical examples, some of them involving anisotropic elasticity and nonquadratic cost functionals.

6.6.8. Energy functionals for elastic medium reconstruction using transient data

Participant: Marc Bonnet.

This work is in collaboration with W. Aquino (Duke Univ., USA). Energy-based misfit cost functionals, known in mechanics as error in constitutive relation (ECR) functionals, are known since a long time to be well suited to (electrostatic, elastic,...) medium reconstruction. In this ongoing work, a transient elastodynamic version of this methodology is developed, with emphasis on its applicability to large time-domain finite element modeling of the forward problem. The formulation involves coupled transient forward and adjoint solutions, which greatly hinders large-scale computations. A computational approach combining an iterative treatment of the coupled problem and the adjoint to the discrete Newmark time-stepping scheme is found to perform well on cases where both the FE model and the identification problem are of large size (2D and 3D elastodynamic numerical experiments made so far involve up to half a million unknown for the discretized inverse problem), making the time-domain ECR functional a worthwhile tool for medium identification.

APICS Project-Team

6. New Results

6.1. Source recovery problems

Participants: Laurent Baratchart, Kateryna Bashtova, Sylvain Chevillard, Juliette Leblond, Dmitry Ponomarev.

This section is concerned with inverse problems for 3-D Poisson-Laplace equations. Though the geometrical settings differ in the 2 sections below, the characterization of silent sources (that give rise to a vanishing potential at measurement points) is one of the common problems to both which has been recently achieved in the magnetization setup, see [14].

6.1.1. Application to EEG

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

In 3-D, functional or clinical active regions in the cortex are often modeled by point-wise sources that have to be localized from measurements on the scalp of a potential satisfying a Laplace equation (EEG, electroencephalography). In the work [3] it was shown how to proceed via best rational approximation on a sequence of 2-D disks cut along the inner sphere, for the case where there are at most 2 sources. Last year, a milestone was reached in the research on the behavior of poles in best rational approximants of fixed degree to functions with branch points [6], to the effect that the technique carries over to finitely many sources (see Section 4.2).

In this connection, a dedicated software "FindSources3D" is being developed, in collaboration with the team Athena and the CMA. We took on this year algorithmic developments, prompted by recent and promising contacts with the firm BESA (see Section 5.6), namely automatic detection of the number of sources (which is left to the user at the moment) and simultaneous processing of data from several time instants. It appears that in the rational approximation step, *multiple* poles possess a nice behavior with respect to branched singularities. This is due to the very physical assumptions on the model (for EEG data, one should consider *triple* poles). Though numerically observed in [8], there is no mathematical justification so far why multiple poles generate such strong accumulation of the poles of the approximants. This intriguing property, however, is definitely helping source recovery. It is used in order to automatically estimate the "most plausible" number of sources (numerically: up to 2, at the moment).

In connection with the work [14] related to inverse magnetization issues (see Section 6.1.2), the characterization of silent sources for EEG has been carried out [42]. These are sums of (distributional) derivatives of Sobolev functions vanishing on the boundary.

In a near future, magnetic data from MEG (magneto-encephalography) will become available along with EEG data; indeed, it is now possible to use simultaneously corresponding measurement devices, in order to measure both electrical and magnetic fields. This should enhance the accuracy of our source recovery algorithms.

Let us mention that discretization issues in geophysics can also be approached by such techniques. Namely, in geodesy or for GPS computations, one is led to seek a discrete approximation of the gravitational potential on the Earth's surface, from partial data collected there. This is the topic of a beginning collaboration with physicist colleagues (IGN, LAREG, geodesy). Related geometrical issues (finding out the geoid, level surface of the gravitational potential) are worthy of consideration as well.

6.1.2. Magnetization issues

This work is carried out in the framework of the "équipe associée Inria" IMPINGE, comprising Eduardo Andrade Lima and Benjamin Weiss from the Earth Sciences department at MIT (Boston, USA) and Douglas Hardin and Edward Saff from the Mathematics department at Vanderbilt University (Nashville, USA),

Localizing magnetic sources from measurements of the magnetic field away from the support of the magnetization is the fundamental issue under investigation by IMPINGE The goal is to determine magnetic properties of rock samples (*e.g.* meteorites or stalactites) from fine field measurements close to the sample that can nowadays be obtained using SQUIDs (supraconducting coil devices). Currently, rock samples are cut into thin slabs and the magnetization distribution is considered to lie in a plane, which makes for a somewhat less indeterminate framework than EEG as regards inverse problems because "less" magnetizations can produce the same field (for the slab has no inner volume).

The magnetization operator is the Riesz potential of the divergence of the magnetization, see (1). Last year, the problem of recovering a thin plate magnetization distribution from measurements of the field in a plane above the sample led us to an analysis of the kernel of this operator, which we characterized in various functional and distributional spaces [14]. Using a generalization of the Hodge decomposition, we were able to describe all magnetizations equivalent to a given one. Here, equivalent means that the magnetizations generate the same field from above and from below if, say, the slab is horizontal. When magnetizations have bounded support, which is the case for rock samples, we proved that magnetizations equivalent from above are also equivalent from below, but this is no longer true for unbounded supports. In fact, even for unidirectional magnetizations, uniqueness of a magnetization generating a given field depends on the boundedness of the support, as we proved that *any* magnetization is equivalent from above to a unidirectional one (with infinite support in general). This helps explaining why methods in the Fourier domain (which essentially loose track of the support information) do encounter problems. It also shows that information on the support must be used in a crucial way to solve the problem.

This year, we produced a fast inversion scheme for magnetic field maps of unidirectional planar geological magnetization with discrete support located on a regular grid, based on discrete Fourier transform [18]. Figures 5 , 6 , 7 and 8 show an example of reconstruction. As the just mentioned article shows, the Fourier approach is computationally attractive but undergoes aliasing phenomena that tend to offset its efficiency. In particular, estimating the total moment of the magnetization sample seems to require data extrapolation techniques which are to take place in the space domain. This is why we have started to study regularization schemes based on truncation of the support in connection with singular values analysis of the discretized problem.

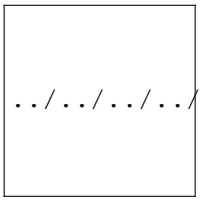


Figure 5. Inria's logo were printed on a piece of paper. The ink of the letters "In" were magnetized along a direction D_1. The ink of the letters "ria" were magnetized along another direction D_2 (almost orthogonal to D_1).

In a joint effort by all members of IMPINGE, we set up a heuristics to recover dipolar magnetizations, using a discrete least square criterion. At the moment, it is solved by a singular value decomposition procedure of the magnetization-to-field operator, along with a regularization technique based on truncation of the support. Preliminary experiments on synthetic data give quite accurate results to recover the net moment of a sample, see the preliminary document http://www-sop.inria.fr/apics/IMPINGE/Documents/NotesSyntheticExample.pdf. We also ran the procedure on real data (measurements of the field generated by Lunar spherules) for which the net moment can be estimated by other methods. The net moment thus recovered matches well the expected moment.

This shows that the technique we use to reduce the support, which is based on thresholding contributions of dipoles to the observations, is capable of eliminating some nearly silent dipole distributions which flaw the

Figure 6. The Z-component of the magnetic field generated by the sample is measured by a SQUID microscope. The measure is performed 200μm above the sample.

Figure 7. The field measured in Figure 6 is inversed, assuming that the sample is uni-dimensionally magnetized along the direction D_1. The letters "In" are fairly well recovered while the rest of the letters is blurred (because the hypothesis about the direction of magnetization is false for "ria").

Figure 8. The field measured in Figure 6 is inversed, assuming that the sample is uni-dimensionally magnetized along the direction D_2. The letters "ria" are fairly well recovered while the rest of the letters is blurred (because the hypothesis about the direction of magnetization is false for "In").

singular value analysis. In order to better understand the geometric nature of such distributions, and thus affirm theoretical bases to the above mentioned heuristics, we raised the question of determining an eigenbasis for the positive self adjoint operator mapping a L^2 magnetization on a rectangle to the field it generates on a rectangle parallel to the initial one. Once ordered according to decreasing eigenvalues, such a basis should retain "as much information as possible" granted the order of truncation.

This is not such an easy problem and currently, in the framework of the PhD thesis of D. Ponomarev, we investigate a simplified two-dimensional analog, defined via convolution of a function on a segment with the Poisson kernel of the upper half-plane and then restriction to a parallel segment in that half-plane. Surprisingly perhaps, this issue was apparently not considered in spite of its natural character and the fact that it makes contact with classical spectral theory. Specifically, it amounts to spectral representation of certain compressed Toeplitz operators with exponential-of-modulus symbols. Beyond the bibliographical research needed to understand the status of this question, only preliminary results have been attained so far.

6.2. Boundary value problems

Participants: Laurent Baratchart, Slah Chaabi, Sylvain Chevillard, Juliette Leblond, Dmitry Ponomarev, Elodie Pozzi.

This work was the occasion of collaborations with Alexander Borichev (Aix-Marseille University), Jonathan Partington (Univ. Leeds, UK), and Emmanuel Russ (Univ. Grenoble, IJF).

6.2.1. Generalized Hardy classes

As we mentioned in Section 4.4 2-D diffusion equations of the form $\mathrm{div}(\sigma\nabla u) = 0$ with real non-negative valued conductivity σ can be viewed as compatibility relations for the so-called conjugate Beltrami equation: $\overline{\partial} f = \nu\overline{\partial f}$ with $\nu = (1-\sigma)/(1+\sigma)$ [4]. Thus, the conjugate Beltrami equation is a means to replace the initial second order diffusion equation by a first order system of two real equations, merged into a single complex one. Hardy spaces under study here are those of this conjugate Beltrami equation: they are comprised of solutions to that equation in the considered domain whose L^p means over curves tending to the boundary of the domain remain bounded. They will for example replace holomorphic Hardy spaces in Problem (P) when dealing with non-constant (isotropic) conductivity. Their traces merely lie in L^p $(1 < p < \infty)$, which is suitable for identification from point-wise measurements, and turn out to be dense on strict subsets of the boundary. This allows one to state Cauchy problems as bounded extremal issues in L^p classes of generalized analytic functions, in a reminiscent manner of what was done for analytic functions as discussed in Section 3.3.1 .

The study of such Hardy spaces for Lipschitz σ was reduced in [4] to that of spaces of pseudo-holomorphic functions with bounded coefficients, which were apparently first considered on the disk by S. Klimentov. Typical results here are that solution factorize as $e^s F$, where F is a holomorphic Hardy function while s is in the Sobolev space $W^{1,r}$ for all $r < \infty$ (Bers factorization), and the analog to the M. Riesz theorem which amounts to solvability of the Dirichlet problem for the initial conductivity equation with L^p boundary data for all $p \in (1, \infty)$. Over the last two years, the case of $W^{1,q}$ conductivities over finitely connected domains, $q > 2$, has been carried out in [13] [61].

In 2013, completing a study begun last year in the framework of the PhD of S. Chaabi, we established similar results in the case where $\log\sigma$ lies in $W^{1,2}$, which corresponds to the critical exponent in Vekua's theory of pseudo-holomorphic functions. This is completely new, and apparently the first example of a solvable Dirichlet problem with L^p boundary data where the conductivity can be both unbounded an vanishing at some places. Accordingly, solutions may also be unbounded inside the domain of the equation, that is, the maximum principle no longer holds. The proof develops a refinement of the Bers factorization based on Muckenhoupt weights and on an original multiplier theorem for $\log W^{1,2}$ functions. A paper on this topic has been submitted [28].

The PhD work of S. Chaabi (defended December 2) contains further work on the Weinstein equation and certain generalizations thereof. This equation results from 2-D projection of Laplace's equation in the presence of rotation symmetry in 3-D. In particular, it is the equation governing the free boundary problem of plasma confinement in the plane section of a tokamak. A method dwelling on Fokas's approach to elliptic boundary value problems has been developed which uses Lax pairs and solves for a Riemann-Hilbert problem on a Riemann surface. It was used to devise semi-explicit forms of solutions to Dirichlet and Neumann problems for the conductivity equation satisfied by the poloidal flux.

In another connection, the conductivity equation can also be regarded as a static Schrödinger equation for smooth coefficients. In particular, a description of laser beam propagation in photopolymers can be crudely approximated by a stationary two-dimensional model of wave propagation in a medium with negligible change of refractive index. In this setting, Helmholtz equation is approximated by a linear Schrödinger equation with one spatial coordinate as evolutionary variable. This phenomenon can be described by a non-stationary model that relies on a spatial nonlinear Schrödinger (NLS) equation with time-dependent refractive index. A model problem has been considered in [20], when the rate of change of refractive index is proportional to the squared amplitude of the electric field and the spatial domain is a plane.

We have also studied composition operators on generalized Hardy spaces in the framework of [13]. In the work [32] submitted for publication, we provide necessary and/or sufficient conditions on the composition map, depending on the geometry of the domains, ensuring that these operators are bounded, invertible, isometric or compact.

6.2.2. Best constrained analytic approximation

Several questions about the behavior of solutions to the bounded extremal problem (P) of Section 3.3.1 have been considered. For instance, truncated Toeplitz operators have been studied in [17], that can be used to quantify robustness properties of our resolution schemes in H^2 and to establish error estimates. Moreover we considered additional interpolation constraints on the disk in Problem (P), and derived new stability estimates for the solution [46]. Such interpolation constraints arise naturally in inverse boundary problems like plasma shaping in last generation tokamaks, where some measurements are performed inside the chamber 4.4 . Of course the version studied so far is much simplified, as it must be carried over to non-constant conductivities and annular geometries.

6.3. Synthesis of compact multiplexers and de-embedding of multiplexers

Participants: Martine Olivi, Sanda Lefteriu, Fabien Seyfert.

This work has been done in collaboration with Stéphane Bila (XLIM, Limoges, France), Hussein Ezzedin (XLIM, Limoges, France), Damien Pacaud (Thales Alenia Space, Toulouse, France), Giuseppe Macchiarella (Politecnico di Milano, Milan, Italy), and Matteo Oldoni (Siae Microelettronica, Milan, Italy).

6.3.1. Synthesis of compact multiplexers

We focused our research on multiplexer with a star topology. These are comprised of a central N-port junction, and of filters plugged on all but common ports (see Figure 9). A possible approach to synthesis of the multiplexer's response is to postulate that each filter channel has to match the multiplexer at n_k frequencies (n_k being the order of the filter) while rejecting the energy at m_k other frequencies (m_k being the order the transmission polynomial of the filter). The desired synthesis can then be cast into computing of a collection of filter's responses matching the energy as prescribed and rejecting it at specified frequencies when plugged simultaneously on the junction. Whether such a collection exists is one of the main open issues facing co-integration of systems in electronics. Investigating the latter led us to consider the simpler problem of matching a filter, on a frequency-varying load, while rejecting energy at fixed specified frequencies. If the order of the filter is n this amounts to fix a given transmission polynomial r and to solve for a unitary polynomial p meeting interpolation conditions of the form:

$$j = 1 \cdots n, \qquad \frac{p}{q}(w_j) = \gamma_j, \ \ |\gamma_j| < 1$$

where q is the unique monic Hurwitz polynomial satisfying the Feldtkeller equation

$$qq^* = pp^* + rr^*.$$

This problem can be seen as an extended Nevanlinna-Pick interpolation problem, which was considered in [65] when the interpolation frequencies lie in the *open* left half-plane. Last year we conjectured the existence and uniqueness of a solution, which were eventually proved true this year when r has no roots on the imaginary axis. We already communicated on the subject (9.1), and a scientific report as well as an article are being written on this result [30]. The proof relies on the local invertibility of an evaluation map that is established using a differential argument and the structure of particular Pick matrices. The case where r has zeros on the imaginary axis is of great interest, and though existence then holds again uniqueness is still not well-understood: it is conjectured that under minor restrictions on the localization of the $\gamma_k' s$ (typically off an algebraic subvariety) the main results still hold.

This research lies at heart of our collaboration with CNES on multiplexer synthesis and the core of the starting ANR project COCORAM on co-integration of filters and antennas (see Section 8.1.1).

6.3.2. De-embedding of multiplexers

Let S be the external scattering parameters of a multiplexer composed of a N-port junction with response T and $N-1$ filters with responses $F_1, \cdots F_{N-1}$ as plotted on Figure 9 . The de-embbeding problem concerns the recovery of the F_k and can be considered under different hypotheses. Last year we studied the de-embedding problem where S and T are known [76] but no particular structure on the F_k is assumed. It was shown that for a generic junction T and for $N > 3$ the de-embedding problem has a unique solution. It was however observed that in practice the junction's response is far from being generic (as it is usually obtained by assembly of smaller T-junctions) which renders the problem extremely sensitive to measurement noise. It was also noticed that in practical applications, scattering measurements of the junction are hardly available.

It was therefore natural to consider following de-embedding problem. Given S the external scattering measurement of the multiplexer, and under the assumptions:

- the F_k are rational of known McMillan degree,
- the coupling geometry of their circuital realization is known,

what can be said about the filter's responses ? It was shown that under the above hypotheses, in particular with no a priori knowledge of T, the filter's responses are identifiable up to a constant chain matrix chained at their second port (nearest to the junction) [24]. It was also shown that this uncertainty bears only on the resonant frequency of the last cavity of each filter, as well as on their output coupling. Most of the filters' important parameters can therefore be recovered. The approach is constructive and relies on rational approximation of certain external scattering parameters, and on an extraction procedure similar to Darlington's synthesis for filters. Software developments have been pursued to implement the latter and practical studies are under way with data furnished by Thales Alenia Space and by Siae Microelettronica. A medium term objective is to extend the Presto-HF (5.3) software to de-embedding problems for multiplexers and more general multi-ports.

This work is pursued in collaboration with Thales Alenia Space, Siae Microelettronica, XLIM and CNES in particular under contract with CNES on compact N-port synthesis (see Section 7.1).

6.4. Detection of the instability of amplifiers

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

This work is conducted in collaboration with Jean-Baptiste Pomet from the McTao team. It is a continuation of a collaboration with CNES and the University of Bilbao.The goal is to help developing amplifiers, in particular to detect instability at an early stage of the design.

Figure 9. Multiplexer made of a junction T and filtering devices $F_1, F_2 \cdots F_N$

Currently, electrical engineers from the University of Bilbao, under contract with CNES (the French Space Agency), use heuristics to diagnose instability before the circuit is physically implemented. We intend to set up a rigorously founded algorithm, based on properties of transfer functions of such amplifiers which belong to particular classes of analytic functions.

In non-degenerate cases, non-linear electrical components can be replaced by their first order approximation when studying stability to small perturbations. Using this approximation, diodes appear as perfect negative resistors and transistors as perfect current sources controlled by the voltages at certain points of the circuit.

In previous years, we had proved that the class of transfer functions which can be realized with such ideal components and standard passive components (resistors, selfs, capacitors and transmission lines) is rather large since it contains all rational functions in the variable and in the exponentials thereof. This makes possible to design circuits that are unstable, although they have no pole in the right half-plane. This remains true even if a high resistor is put in parallel of the circuit, which is rather unusual. These pathological examples are unrealistic, though, because they assume that non-linear elements continue to provide gain even at very high frequencies. In practice, small capacitive and inductive effects (negligible at moderate frequencies) make these components passive for very high frequencies.

In 2013, we showed that under this simple assumption that there are small inductive and capacitive effects in active components, the class of transfer functions of realistic circuits is much smaller than in previous situation. Our main result is that a realistic circuit is unstable if and only if it has poles in the right half-plane. Moreover, there can only be finitely many of them. Besides this result, we also generalized our description of the class of transfer functions achievable with ideal components, to include the case of transmission lines with loss. An article is currently being written on this subject.

6.5. Rational and meromorphic approximation

Participants: Laurent Baratchart, Sylvain Chevillard.

This work has been done in collaboration with Herbert Stahl (Beuth-Hochsch.), Maxim Yattselev (Purdue Univ. at Indianapolis, USA), Tao Qian (Univ. Macao).

We published last year an important result in approximation theory, namely the counting measure of poles of best H^2 approximants of degree n to a function analytically continuable, except over finitely many branchpoints lying outside the unit disk, converges to the Green equilibrium distribution of the compact set of minimal Green capacity outside of which the function is single valued [6] (see also [21]). This result warrants source recovery techniques used in Section 6.1.1 . We considered this year a similar problem for best uniform meromorphic approximants on the unit circle (so-called AAK approximants after Adamjan, Arov and Krein), in the case where the function may have poles and essential singularities. The technical difficulties are considerable, and though a line of attack has been adopted we presently struggle with the proof.

We also studied partial realizations, or equivalently Padé approximants to transfer functions with branchpoints. Identification techniques based on partial realizations of a stable infinite-dimensional transfer function are known to often provide unstable models, but the question as to whether this is due to noise or to intrinsic instability was not clear. This year, we published a paper showing that, in the case of 4 branchpoints, the pole behavior generically has deterministic chaos to it [15].

We also considered the issue of lower bounds in rational approximation. Prompted by renewed interest for linearizing techniques such as vector fitting in the identification community, we studied linearized errors in light of the topological approach in [51], to find that, when properly normalized, they give rise to lower bounds in L^2 rational approximation. Moreover, these make contact with AAK theory which furnishes more, easily computable lower bounds. This is an interesting finding, for lower bounds are usually difficult to get in approximation and though quite helpful to get an appraisal of what can be hoped for in modeling. Dwelling on this, we established for the first time lower bounds in L^2 rational approximation to some badly L^∞ approximable functions (Blaschke products) and showed equivalence, up to a constant, of best L^2 and L^∞ approximation to functions with branchpoints (such as those appearing in inverse source problems for

EEG, see Section 6.1.1). An article on this subject is currently submitted for publication in the Journal of Approximation Theory [29].

6.6. Tools for numerically guaranteed computations

Participant: Sylvain Chevillard.

The overall and long-term goal is to enhance the quality of numerical computations. The progress made during year 2013 is the following:

- Publication of a work with Marc Mezzarobba (who was with Aric project-team at that time, and who is now with LIP6) about the efficient evaluation of the Airy $\mathrm{Ai}(x)$ function when x is moderately large [22]. The Taylor series of the Airy Ai function (as many others such as, e.g., Bessel functions or erf) is ill-conditioned when x is not small. To overcome this difficulty, we extend a method by Gawronski, Müller and Reinhard, known to solve the issue in the case of the error function erf. We rewrite $\mathrm{Ai}(x)$ as $G(x)/F(x)$ where F and G are two functions with well-conditioned series. However, the coefficients of G turn out to obey a three-terms ill-conditioned recurrence. We evaluate this recurrence using Miller's backward algorithm with a rigorous error analysis. Function Ai is an example, but ideally the process could be automated to handle some appropriate class of functions in a future work.
- A more general endeavor is to develop a tool that helps developers of libms in their task. This is performed by the software Sollya [3], developed in collaboration with C. Lauter (Université Pierre et Marie Curie) and M. Joldeş (LAAS). In 2013, we released version version 4.0 (in May) and 4.1 (in November) of Sollya. Among other things these releases make available to the user all features of Sollya as a C library. They also introduce the possibility of computing Chebyshev models, and a generalization of Remez algorithm allowing the user to compute a L^∞ best approximation of a real-valued function on a bounded real interval by any linear combination of given functions.

[3] http://sollya.gforge.inria.fr/

BIPOP Project-Team

6. New Results

6.1. Multiple impacts modelling

Participants: Bernard Brogliato, Ngoc-Son Nguyen.

The work consists of studying two systems: the rocking block and tapered chains of balls, using the Darboux-Keller model of multiple impacts previously developed. The objectives are threefold: 1) show that the model predicts well the motion by careful comparisons with experimental data found in the literature, 2) study the system's dynamics and extract critical kinetic angles that allow the engineer to predict the system's gross motion, 3) develop numerical code inside the SICONOS platform that incorporates the model of multiple impact. The influence of the kinetic angles in the rocking block motion with friction is analysed as well, numerically. Extensive experimental works have been conducted by our colleague C. Liu at PKU on a disc-ball system. Results are in [30], [24] [64], and in the monograph [15]. Another work is dedicated to analysing the influence of bilateral holonomic constraints on the well-posedness of the complementarity problem obtained from the (frictionless) unilateral constraints. Gauss' principle extension to this case is also analysed [22].

6.2. Discrete-time sliding mode control

Participants: Vincent Acary, Bernard Brogliato, Olivier Huber, Bin Wang.

This topic concerns the study of time-discretized sliding-mode controllers. Inspired by the discretization of nonsmooth mechanical systems, we propose implicit discretizations of discontinuous, set-valued controllers. This is shown to result in preservation of essential properties like simplicity of the parameters tuning, suppression of numerical chattering, reachability of the sliding surface after a finite number of steps, and disturbance attenuation by a factor h or h^2 [36]. This work is part of the ANR project CHASLIM. Within the framework of CHASLIM we have performed many experimental validations on the electropneumatic setup of IRCCyN (Nantes), which nicely confirm our theoretical and numerical predictions: the implicit implementation of sliding mode control, drastically improves the input and output chattering behaviours. In particular the high frequency bang-bang controllers which are observed with explicit discretizations, are completely suppressed.

6.3. Dissipativity preserving methods

Participants: Vincent Acary, Bernard Brogliato.

This work concerns the analysis of so-called theta-methods applied to linear complementarity systems that are dissipative (in the sense of Willems). Necessary and sufficient conditions for dissipativity preservation after the time-discretization are derived (preservation of the storage function, the supply rate and the dissipation function). The possible state jumps are also analyzed [57]. It is shown that excepted when the system is state lossless and theta = 0.5, the conditions for dissipativity preservation are very stringent. In this article we also provide (for the first time, to the best of our knowledge) a rigorous definition of numerical dissipation, which remained until now a vague notion in numerical analysis.

6.4. Lur'e set-valued dynamical systems

Participants: Bernard Brogliato, Aneel Tanwani, Christophe Prieur.

Lur'e systems are quite popular in Automatic Control since the fifties. Set-valued Lur'e systems possess a static feedback nonlinearity that is a multivalued function. This study consists in the mathematical analysis (existence and uniqueness of solutions) and the stability analysis (Lyapunov stability, invariance principle) of classes of set-valued Lur'e systems, with applications in complementarity dynamical systems, relay systems, mechanical systems with dry friction, electrical circuits, etc. Our works in this field started in [51]. The results in [53] extend those in [52] with an accurate characterization of the maximal monotonicity of the central operator of these systems, which consists of a projection-like operator. Concrete and verifiable criteria are provided for the above classes (complementarity, relay systems). Results on state observers for classes of Lur'e systems (namely: Moreau's sweeping process of first and second order, and with prox-regular sets) are proposed in [47], [39]. Therein the convexity is replaced by the far more general notion of prox-regularity, which destroys the monotonicity.

6.5. Analysis of Limit Cycles in Piecewise Linear Systems

Participants: Vincent Acary, Bernard Brogliato, Valentina Sessa.

Autonomous piecewise linear systems in the Lur'e form may exhibit periodic steady-state oscillations. For many practical systems belonging to this class the period and the shape of the oscillation is difficult to be predicted a priori. In this work the complementarity approach is used to tackle the issue. The complementarity formalism is used to represent the closed-loop system and a phase condition acting as an anchor equation for the periodic solution. By discretizing the dynamics a mixed complementarity problem is formulated. The corresponding solution provides an accurate prediction of the steady-state oscillation and its period. Numerical results show the effectiveness of the proposed technique for the computation of stable and sliding periodic solutions. The analysis of the steady-state solution of a Colpitts oscillator is considered as an illustration. This work has been presented at CDC 2013 in [37].

6.6. Simulation and stability of piecewise linear gene networks

Participants: Vincent Acary, Arnaud Tonnelier, Bernard Brogliato.

This work has been done in collaboration with the IBIS project team, it is reported in [45], [19]. Gene regulatory networks control the response of living cells to changes in their environment. A class of piecewise-linear (PWL) models, which capture the switch-like interactions between genes by means of step functions, has been found useful for describing the dynamics of gene regulatory networks. The step functions lead to discontinuities in the right-hand side of the differential equations. This has motivated extensions of the PWL models based on differential inclusions and Filippov solutions, whose analysis requires sophisticated numerical tools. We present a method for the numerical analysis of one proposed extension, called Aizerman-Pyatnitskii (AP)-extension, by reformulating the PWL models as a mixed complementarity system (MCS). This allows the application of powerful methods developed for this class of nonsmooth dynamical systems, in particular those implemented in the Siconos platform. We also show that under a set of reasonable biological assumptions, putting constraints on the right-hand side of the PWL models, AP-extensions and classical Filippov (F)-extensions are equivalent. This means that the proposed numerical method is valid for a range of different solution concepts. We illustrate the practical interest of our approach through the numerical analysis of three well-known networks developed in the field of synthetic biology.

In addition, we have investigated oscillatory regimes in repressilator-type models with piecewise linear dynamics [48]. We derived exact analytical conditions for oscillations and showed that the relative location between the dissociation constants of the Hill functions and the ratio of kinetic parameters determines the possibility of oscillatory activities. We also computed analytically the probability of oscillations. Results suggest that a switch-like coupling behaviour, a time-scale separation and a repressilator-type architecture with an even number of elements facilitate the emergence of sustained oscillations in biological systems.

6.7. Numerical analysis and simulation of mechanical systems with constraints

6.7.1. Event-capturing schemes for nonsmooth mechanical systems

Participant: Vincent Acary.

To perform the numerical time integration of nonsmooth mechanical systems, the family of event-capturing time–stepping schemes are the most robust and efficient tools. Nevertheless, they suffer from several drawbacks : a) a low–order accuracy (at best at order one), b) a drift phenomena when the unilateral constraints are treated at the velocity level and c) a poor "energetic" behavior in terms of stabilizing the high–frequency dynamics. We proposed self-adapting schemes by applying time–discontinuous Galerkin methods to the measure differential equation in [31]. In order to satisfy in discrete time, the impact law and the constraints at the position and the velocity level, an adaptation of the well-known Gear–Gupta–Leimkuhler approach has been developed in [18]. Finally, the energetic behavior of the standard Moreau–Jean scheme has been addressed in [26] by developing a Newmark–type scheme for nonsmooth dynamics.

6.7.2. Numerical time–integration methods for event-detecting schemes.

Participants: Vincent Acary, Bernard Brogliato, Mounia Haddouni.

The CIFRE thesis of M. Haddouni concerns the numerical simulation of mechanical systems subject to holonomic bilateral constraints, unilateral constraints and impacts. This work is performed in collaboration with ANSYS and the main goal is to improve the numerical time–integration in the framework of event-detecting schemes. Between nonsmooth events, time integration amounts to numerically solving a differential algebraic equations (DAE) of index 3. We have compared dedicated solvers (Explicit RK schemes, Half-explicit schemes, generalizes α-schemes) that solve reduced index formulations of these systems. Since the drift of the constraints is crucial for the robustness of the simulation through the evaluation of the index sets of active contacts, we have proposed some recommendations on the use of the solvers of dedicated to index-2 DAE. This work has been presented in [35], [40].

6.7.3. Multibody systems woth contact, friction and clearances

Participants: Vincent Acary, Bernard Brogliato, Narendra Akadkhar.

The PhD thesis of N. Akadkhar under contract with Schneider Electric concerns the numerical simulation of mechanical systems with unilateral constraints and friction, where the presence of clearances in imperfect joints plays a crucial role. A first work deals with four-bar planar mechanisms with clearances at the joints, which induce unilateral constraints and impacts, rendering the dynamics nonsmooth. The objective is to determine sets of parameters (clearance value, restitution coefficients, friction coefficients) such that the system's trajectories stay in a neighborhood of the ideal mechanism (*i.e.* without clearance) trajectories. The analysis is based on numerical simulations obtained with the projected Moreau-Jean time-stepping scheme. These results have been submitted to the ENOC 2014 conference. It is planned to extend these simulations to frictional cases and to mechanisms of circuit breakers.

6.8. Mechanical rods

6.8.1. High-order models of mechanical rods

Participants: Florence Bertails-Descoubes, Romain Casati.

Reduced-coordinate models for rods such as the articulated rigid body model or the super-helix model [50] are able to capture the bending and twisting deformations of thin elastic rods while strictly and robustly avoiding stretching deformations. In this work we are exploring new reduced-coordinate models based on a higher-order geometry. Typically, elements are defined by a polynomial curvature function of the arc length, of degree $d \geq 1$. The main difficulty compared to the super-helix model (where $d = 0$) is that the kinematics has no longer a closed form. Last year, in R. Casati's PhD's thesis, we extended this result to the full 3D case. The key idea was to integrate the rod's kinematics using power series expansion, and to design an accurate and efficient computational algorithm adapted to floating point arithmetics. Our method nicely propagates to the computation of the full dynamic of a linked chain of 3d clothoid. This year we thoroughly compared our methods against other rod models from the literature, in terms of both accuracy and computational efficiency. Our results demonstrate that our model is competitive compared to former models, and yields a better trade-off in the case of highly curly rods. All these results were published and presented this year at SIGGRAPH [25]. The source code is also freely distributed under a GPLv.3 license (see Section 5.3).

6.8.2. Inverse modeling of mechanical rods subject to frictional contact

Participants: Florence Bertails-Descoubes, Alexandre Derouet-Jourdan, Gilles Daviet.

Controlling the input shape of slender structures such as rods is desirable in many design applications (such as hairstyling, reverse engineering, etc.), but solving the corresponding inverse problem is not straightforward. In [54], [55] we noted that reduced-coordinates models such as the super-helix are well-suited for static inversion in presence of gravity.

We are facing two main difficulties: 1/ the geometrical fitting of a piecewise helix to an arbitrary input curve and 2/ the inversion a super-helix subject to gravity *and* contacting forces.

6.8.2.1. Geometrical fitting: from an arbitrary smooth curve to a C^1 piecewise helix

Participants: Florence Bertails-Descoubes, Alexandre Derouet-Jourdan.

In A. Derouet-Jourdan's PhD's thesis (co-supervised by Joëlle Thollot, EPI Maverick), we solved this problem by extending to 3d the floating tangents algorithm introduced in 2d in [54]. In this new method, only tangents are strictly interpolated while points are displaced in an optimal way so as to lie in a feasible configuration, *i.e.*, a configuration that is compatible with the interpolation by a helix. Our approach relies upon the co-helicity condition found by Ghosh [56], which was however only partially proved in [56]. To ensure the existence of the helix and prove its uniqueness in the general case, we complete the proof which serves as the basis for our reconstruction algorithm.

Our method proves to be efficient and robust as it can successfully handle large and complex datasets from real curve aquisitions, such as the capture of hair fibers or the magnetic field of a star. We also compared our method against a standard nonlinear least-squares methods. Unlike the optimization approach which often fail to converge in the case of frizzy input curves, our method remains extremely fast regardless the complexity of the input curves. The set of these results was published this year at Computer-Aided Geometric Design [28]. This work has been transferred to L'Oréal in December 2013. Some source code is also freely released for academics under the GPLv.3 license (see Section 5.3).

6.8.2.2. Inverse modeling of a super-helix assembly subject to frictional contact

Participants: Florence Bertails-Descoubes, Alexandre Derouet-Jourdan, Gilles Daviet.

In A. Derouet-Jourdan's PhD's thesis (co-supervised by Joëlle Thollot, EPI Maverick), we bring a first solution to the challenging problem consisting in identifying the intrinsic geometry of a fiber assembly under gravity and (unknown) frictional external and mutual contacts, from a single configuration geometry (a set of geometric curves). Taking an arbitrary fiber assembly geometry (such as hair) as input together with corresponding interacting meshes (such as the body mesh), we interpret the fiber assembly shape as a static equilibrium configuration of a fiber assembly simulator, in the presence of gravity as well as fiber-mesh and fiber-fiber frictional contacts. Assuming fibers parameters are homogeneous and lie in a plausible range of physical values, we show that this large, underdetermined inverse problem can be formulated as a well-posed constrained optimization problem (second-order cone quadratic program), which can be solved robustly and efficiently by leveraging the frictional contact solver of our direct simulator for fiber assemblies [8]. Our method was successfully applied to the animation of various hair geometries, ranging from synthetic hairstyles manually designed by an artist to the most recent human hair data reconstructed from capture. These results were published this year at SIGGRAPH Asia [27].

6.9. Threshold in neural models

Participant: Arnaud Tonnelier.

We studied the threshold for spike initiation in two-dimensionnal neural models. A threshold criterion that depends on both membrane voltage and recovery (or adaptation) variable is proposed. Our approach provides a simple and unified framework that can account for adapting threshold, threshold variability, dynamic threshold, inhibition-induced spike and postinhibitory facilitation. Implications on neural modeling and on neural dynamics are discussed.

6.10. Nonsmooth modes in chains of impact oscillators

Participants: Vincent Acary, Guillaume James, Franck Pérignon.

Chains of impact oscillators arise for example as finite-element models of thin oscillating mechanical structures (a string under tension or a clamped beam) contacting rigid obstacles. Nonlinear periodic waves are observed in experiments on such systems, but relatively little is known from a theoretical point of view on their existence and stability. In 2008, Gendelman and Manevitch have analyzed the existence and stability of nonlinear localized modes (breathers) for discrete linear chains with a single node undergoing rigid impacts. In this work, we introduce a numerical method allowing to compute branches of time-periodic solutions when an arbitrary number of nodes undergo rigid impacts without energy dissipation. For this purpose, we reformulate the search of periodic solutions as a boundary value problem incorporating unilateral constraints. We illustrate this numerical approach by computing different families of breathers and nonlinear normal modes. Our method is much more effective than a numerical continuation of periodic solutions based on compliant models, which requires to integrate stiff differential equations and lead to costly numerical continuation. These results have been submitted to the ENOC 2014 conference.

6.11. Traveling waves in spatially discrete excitable media

Participants: José Eduardo Morales, Arnaud Tonnelier, Guillaume James.

The propagation of traveling waves in excitable media is a widespread phenomenon, with applications ranging from forest fires to electrical signals propagating along nerve fibers. The case of spatially discrete excitable models is notoriously difficult to analyze. In particular, for the discrete FitzHugh-Nagumo reaction-diffusion system, the existence of pulses for a general class of bistable nonlinearities has been proved only recently (Hupkes and Sandstede, 2010). The existence of pulses under more general types of interactions (e.g. elastic instead of diffusive) remains an open question, as well as traveling wave propagation in higher-dimensional systems. These problems will be tackled in the PhD thesis of J.-E. Morales (advisors A. Tonnelier and G. James), which started on November 2013. J.-E. Morales has started to analyze pulse propagation in the excitable Burridge-Knopoff model, which finds applications in the context of nonlinear friction. This model includes elastic interactions between particles, and an additional difficulty linked with nonsmoothness of the (multivalued) Coulomb friction law.

6.12. Nonlinear waves in granular chains

Participants: Guillaume James, Bernard Brogliato, Ngoc-Son Nguyen.

Granular chains made of aligned beads interacting by contact (e.g. Newton's cradle) are widely studied in the context of impact dynamics and acoustic metamaterials. When a large number of beads are present, their dynamics can be described by infinite-dimensional differential equations, which possess a limited smoothness when unilateral Hertzian contact interactions are considered. In this context, we have developed and analyzed new reduced-order models describing nonlinear wave propagation in such systems. In the work [49] (collaboration with D.Pelinovsky, McMaster Univ.), we analyze small amplitude slowly modulated compression waves in the limit when the exponent of the Hertz force is close to unity. From a multiple scale analysis, we derive a new type of Korteweg-de Vries equation with logarithmic nonlinearity allowing to approximate wave profiles, in particular solitary wave solutions.

In addition the LZB model introduced in [14] has been extensively used to numerically investigate wave phenomena in chains of aligned balls (tapered, monodisperse, anti-tapered, stepped chains). Thorough comparisons with experimental results reported in the Granular Matter literature have been made. The results are reported in the monograph [15].

6.13. Robotics

6.13.1. Lexicographic Least-Squares solver

Participants: Pierre-Brice Wieber, Dimitar Dimitrov.

We have been working on Multi-Objective Least-Squares problems with inequality constraints for the last few years, focusing especially on the Lexicographic case. A previous collaboration with LAAS-CNRS and CEA-LIST led to the development of a software, SOTH , based on Complete Orthogonal Decompositions, which has become a *de facto* reference in robotics when controlling robots (mobile, manipulator or humanoid) through constraints. The focus this year in the Bipop team has been to accelerate computations by reworking the inner matrix decomposition by combining QR and LU decompositions. The resulting solver, called LexLS, is approximately 5 times faster than the previous SOTH solver on most problems. But the main result has been to show both in theory and practice that it is faster to solve a Lexicographic problem than a Weighted problem, on the contrary to popular beliefs both in robotics and optimization theory. That leads to a reversal of popular approaches that prefer to solve weighted problems (thought to be faster to solve) as approximations to lexicographic problems (thought to be slower to solve).

6.13.2. Mobile manipulation by humanoid robots

Participants: Pierre-Brice Wieber, Dimitar Dimitrov, Alexander Sherikov, Jory Lafaye.

The realization of mobile manipulation by humanoid robots requires the handling of two simultaneous problems: taking care of the dynamic balance of the robot, what is usually done with Model Predictive Control (MPC) schemes, and redundant motion and force control of the whole body of the robot, what is usually done with a Quadratic Program, or a more advanced Lexicographic Least-Squares problem (see above). These two problems are usually solved in sequence: an MPC scheme first computes the necessary motion of the feet and Center of Mass (CoM) of the robot, then motion and force redundancy of the whole body of the robot is resolved. We have observed that this sequence corresponds to a lexicographic order between two objectives, feet and CoM motion first, the rest of the body after, which limits the possibility to tackle scenarios where we would like the motion of the CoM of the robot to be driven by the motion of the rest of the body of the robot, for example to catch an object with the hand. We have proposed therefore to reorganize the order between these different objectives, building on the LexLS solver presented above.

6.13.3. Reactive trajectory generation

Participants: Pierre-Brice Wieber, Dimitar Dimitrov, Saed Al Homsy, Matthieu Guilbert.

The goal of the ongoing collaboration with Adept Technologies is to generate near time optimal trajectories in the presence of moving obstacles in real time. Results are not public yet due to industrial constraints.

6.14. Optimization

6.14.1. Semidefinite programming and combinatorial optimization

Participant: Jérôme Malick.

We have worked with Frederic Roupin (Prof. at Paris XIII) and Nathan Krislock (Assistant Prof. at North Illinois University, USA) on the use of semidefinite programming to solve combinatorial optimization problems to optimality.

We proposed a new family of semidefinite bounds for 0-1 quadratic problems with linear or quadratic constraints [61]. We have embedded the new bounds within branch-and-bound algorithms to solve 2 standard combinatorial optimization problems to optimality.

- *Max-cut.* We developed [60] an improved bounding procedure obtained by reducing two key parameters (the target level of accuracy and the stopping tolerance of the inner Quasi-Newton engine) to zero, and iteratively adding triangle inequality cuts. We also precisely analyzed its theoretical convergence properties. We show that our method outperform the state-of-the-art solver ([62]) on the large test-problems.
- *Heaviest k-subgraph problems*. Adapting the techniques we developped for the max-cut problem, we have proposed in [59] an big improvement of the first algorithm (up to 10 times faster). For the first time, we were able to solve exactly k-cluster instances of size 160. In practice, our method works particularly fine on the most difficult instances (with a large number of vertices, small density and small k).

We have also been working on a generic online semidefinite-based solver for binary quadratic problems using the generality of [61]. Finally, a first web interface for our solvers and our data sets are available online at http://lipn.univ-paris13.fr/BiqCrunch/.

6.14.2. On computing marginal prices in electricity production

Participants: Jérôme Malick, Sofia Zaourar.

Unit-commitment optimization problems in electricity production are large-scale, nonconvex and heterogeneous, but they are decomposable by Lagrangian duality. Realistic modeling of technical production constraints makes the dual objective function computed inexactly though. An inexact version of the bundle method has been dedicated to tackle this difficulty [58]. We have worked on two projects related to solving dual unit-commitment problem by inexact bundle methods.

- *Stabilization.* We observed that the computed optimal dual variables show a noisy and unstable behaviour, that could prevent their use as price indicator. We have proposed a simple and controllable way to stabilize the dual optimal solutions, by penalizing the total variation of the prices [63]. Our illustrations on the daily electricity production optimization of EDF show a strinking stabilization at a negligible cost.
- *Acceleration*. We have worked with Welington Oliveira (IMPA, Brazil) on the acceleration of inexact bundle methods by taking advantage of cheap-to-get inexact information on the objective function which comes without any tighness guarantee though. We came up with a new family of bundle methods incorporating this coarse inexact information, to get better iterates. We have studied the convergence of these method and we have conducted numerical experimentation on unit-commitment problems and on two-stage linear problems show a subtantial gain in the overall computing time. This research is about to be released in a preprint in HAL

COMMANDS Project-Team

5. New Results

5.1. Optimality conditions in Pontryagin form for optimal control problems

Participants: Joseph Frédéric Bonnans, Xavier Dupuis, Laurent Pfeiffer.

5.1.1. Necessary conditions

In the paper [31], we state and prove first- and second-order necessary conditions in Pontryagin form for optimal control problems with pure state and mixed control-state constraints. We say that a Lagrange multiplier of an optimal control problem is a Pontryagin multiplier if it is such that Pontryagin's minimum principle holds, and we call optimality conditions in Pontryagin form those which only involve Pontryagin multipliers. Our conditions rely on a technique of partial relaxation, and apply to Pontryagin local minima.

5.1.2. Sufficient conditions

In the paper [32], we consider sufficient conditions. More precisely, given a reference feasible trajectory of an optimal control problem, we say that the quadratic growth property for bounded strong solutions holds if the cost function of the problem has a quadratic growth over the set of feasible trajectories with a bounded control and with a state variable sufficiently close to the reference state variable. Our sufficient second-order optimality conditions in Pontryagin form ensure this property and ensure *a fortiori* that the reference trajectory is a bounded strong solution. Our proof relies on a decomposition principle, which is a particular second-order expansion of the Lagrangian of the problem.

5.1.3. Shooting Approach to Optimal Control Problems

Participant: Joseph Frédéric Bonnans.

In the paper [24] we give an overview of the shooting technique for solving deterministic optimal control problems. This approach allows to reduce locally these problems to a finite dimensional equation. We first recall the basic idea, in the case of unconstrained or control constrained problems, and show the link with second-order optimality conditions and the analysis or discretization errors. Then we focus on two cases that are now better understood: state constrained problems, and affine control systems. We end by discussing extensions to the optimal control of a parabolic equation.

5.2. Applications of deterministic optimal control problems

5.2.1. Optimization of running strategies based on anaerobic energy and variations of velocity

Participant: Joseph Frédéric Bonnans.

In the report [29] we present new models, numerical simulations and rigorous analysis for the optimization of the velocity in a race. In a seminal paper, Keller [74], [75] explained how a runner should determine his speed in order to run a given distance in the shortest time. We extend this analysis, based on the equation of motion and aerobic energy, to include a balance of anaerobic energy (or accumulated oxygen deficit) and an energy recreation term when the speed decreases. We also take into account that when the anaerobic energy gets too low, the oxygen uptake cannot be maintained to its maximal value. Using optimal control theory, we obtain a proof of Keller's optimal race, and relate the problem to a relaxed formulation, where the propulsive force represents a probability distribution rather than a value function of time. Our analysis leads us to introduce a bound on the variations of the propulsive force to obtain a more realistic model which displays oscillations of the velocity. Our numerical simulations qualitatively reproduce quite well physiological measurements on real runners. We show how, by optimizing over a period, we recover these oscillations of speed. We point out that our numerical simulations provide in particular the exact instantaneous anaerobic energy used in the exercise.

5.2.2. Optimal control of leukemic cell population dynamics

Participant: Xavier Dupuis.

In the paper [33] we discuss the optimal co-administration of two drugs for some acute myeloid leukemias (AML), and we are looking for in vitro protocols as a first step. This issue can be formulated as an optimal control problem. The dynamics of leukemic cell populations in culture is given by age-structured partial differential equations, which can be reduced to a system of delay differential equations, and where the controls represent the action of the drugs. The objective function relies on eigenelements of the uncontrolled model and on general relative entropy, with the idea to maximize the efficiency of the protocols. The constraints take into account the toxicity of the drugs. We present in this paper the modeling aspects, as well as theoretical and numerical results on the optimal control problem that we get.

5.2.3. Contrast imaging problem in nuclear magnetic resonance

Participant: Pierre Martinon.

In collaboration with team McTAO (Sophia), we studied in [25] and [36] the contrast imaging problem in nuclear magnetic resonance, modeled as Mayer problem in optimal control. The optimal solution can be found as an extremal, solution of the Maximum Principle and analyzed with the techniques of geometric control. A first synthesis of locally optimal solutions is given in the single-input case, with some preliminary results in the bi-input case. We conducted a comprehensive numerical investigation of the problem, using a combination of indirect shooting (HAMPATH software) and direct method (BOCOP), with a moment-based (LMI) technique to estimate the global optimum.

Figure 2. Contrast in quantum control for NMR - Oxygenated / deoxygenated blood

5.2.4. Optimizing the anaerobic digestion of microalgae in a coupled process

Participant: Pierre Martinon.

In collaboration with the Inra-Inria team MODEMIC (Montpellier), we studied in [30] a bio-reactor system describing the coupling of a culture of micro-algae and an anaerobic digester. Our aim is to optimize the production of methane in the digester during a certain number of days with respect to the dilution rate (the input flow of micro-algae in the digester). The mathematical model for the dynamics of the two reactors takes into account a periodic day-night model of the light in the culture of micro-algae, and a chemostat model for the digester. We first prove existence and attraction of periodic solutions for a one day period, and we apply Pontryagin's Maximum Principle (PMP) in order to characterize optimal controls. We provide numerical simulations for different light models, by a direct method that we refine using an indirect shooting. We also investigate the dependence of the optimal cost with respect to the ratio of the volumes of the two tanks. Finally, we investigate the optimal strategies over a large number of days without periodic constraints, and compared the mean cost to the optimal cost over one period.

Figure 3. Coupled bio-reactor for micro-algae digestion - Attraction property

5.2.5. Design of optimal experiments for parameter estimation of microalgae growth models

Participant: Pierre Martinon.

In collaboration with team BIOCORE (Sophia), we investigated in [27] techniques of Optimal Experiment Design for microalgae growth models. In order to have microalgae growth models that are useful for prediction and process optimization, reliable parameters need to be provided. This reliability implies a careful design of experiments that can be exploited for parameter estimation. OED techniques can provide guidelines for the design of experiments with high informative content that allow an accurate parameter estimation. We study a real experimental device devoted to evaluate the effect of temperature and light on microalgae growth. On the basis of a mathematical model of the experimental system, the optimal experiment design problem was solved

as an optimal control problem. E-optimal experiments were obtained by using two discretization approaches, namely sequential and simultaneous. The results showed that an adequate parameterization of the experimental inputs provided optimal solutions very close to those provided by the simultaneous discretization. Simulation results showed the relevance of determining optimal experimental inputs for achieving an accurate parameter estimation.

Figure 4. Experimental apparatus for the study of micro-algae growth (Ifremer)

5.2.6. Controllability and optimal strokes for N-link microswimmer

Participant: Pierre Martinon.

In [39] we focus on the N-link swimmer, a generalization of the classical Purcell swimmer. We use the simplification of the Resistive Force Theory to derive the motion equation for the swimmer in a fluid with a low Reynolds number. We prove that the swimmer is controllable in the whole plane when it is composed by more than 3 sticks and for almost every set of stick lengths. As a direct result, we show that there exists an optimal swimming strategy which leads to minimize the time to reach a desired configuration. Numerical experiments on the case of the Purcell swimmer suggest that the optimal strategy is periodic, i.e. composed of a sequence of identical strokes. Our results indicate that this candidate for an optimal stroke indeed gives a better speed than the classical Purcell stroke. Future directions for this work include the design of robotic micro-swimmers, as well as investigation of the movement of swimming micro-organisms.

5.3. Hamilton-Jacobi (HJ) approach

5.3.1. Dynamic programming and error estimates for stochastic control with Max cost

Participants: Olivier Bokanowski, Athena Picarelli, Hasnaa Zidani.

Figure 5. Purcell (3-link) swimmer - Purcell vs optimal stroke

The paper [35] is concerned with stochastic optimal control for a running maximum cost. A direct approach based on dynamic programming techniques is studied leading to the characterization of the value function as the unique viscosity solution of a second order Hamilton-Jacobi-Bellman (HJB) equation with an oblique derivative boundary condition. A general numerical scheme is proposed and a convergence result is provided. Error estimates are obtained for the semi-Lagrangian scheme. These results can apply to the case of lookback options in finance. Moreover, optimal control problems with maximum cost arise in the characterization of the reachable sets for a system of controlled stochastic differential equations. Some numerical simulations on examples of reachable analysis are included to illustrate our approach.

5.3.2. Optimal feedback control of undamped wave equations by solving a HJB equation

Participant: Hasnaa Zidani.

An optimal finite-time horizon feedback control problem for (semi linear) wave equations is studied in [42]. The feedback law can be derived from the dynamic programming principle and requires to solve the evolutionary Hamilton-Jacobi-Bellman (HJB) equation. Classical discretization methods based on finite elements lead to approximated problems governed by ODEs in high dimensional space which makes infeasible the numerical resolution by HJB approach. In the present paper, an approximation based on spectral elements is used to discretize the wave equation. The effect of noise is considered and numerical simulations are presented to show the relevance of the approach

5.3.3. Transmission conditions on interfaces for Hamilton-Jacobi-Bellman equations

Participants: Hasnaa Zidani, Zhiping Rao.

The works [43], [28] deal with deterministic control problems where the dynamic and the running cost can be completely different in two (or more) complementary domains of the space $I\!R^N$. As a consequence, the dynamics and running cost present discontinuities at the interfaces of these domains. This leads to a complex interplay that has to be analyzed among transmission conditions to "glue" the propagation of the value function on the interfaces. Several questions arise: how to define properly the value function(s) and what is (are) the right Bellman Equation(s) associated with this problem?. In the case of a simple geometry (namely when the space $I\!R^N$ is partitioned into two subdomains separated with an interface which is assumed to be a regular hypersurface without any connectedness requirement), [43] discuss different conditions on the hyperplane where the dynamic and the running cost are discontinuous, and the uniqueness properties of the Bellman problem are studied. In this paper it is used a dynamical approach, namely instead of working with test functions, the accent is put on invariance properties of an augmented dynamics related to the integrated control system. The comparison principle is accordingly based, rather than on (semi)continuity of the Hamiltonian appearing in the Hamilton–Jacobi–Bellman equation, on some weak separation properties of this dynamics with respect to the stratification. A more general situation where the space is partionned on several domains is also analyzed in [28].

5.3.4. Singular perturbation of optimal control problems on multi-domains

Participants: Nicolas Forcadel, Hasnaa Zidani.

The goal of the paper[38] is to study a singular perturbation problem in the framework of optimal control on multi-domains. We consider an optimal control problem in which the controlled system contains a fast and a slow variables. This problem is reformulated as an Hamilton-Jacobi-Bellman (HJB) equation. The main difficulty comes from the fact that the fast variable lives in a multi-domain. The geometric singularity of the multi-domains leads to the discontinuity of the Hamiltonian. Under a controllability assumption on the fast variables, the limit equation (as the velocity of the fast variable goes to infinity) is obtained via a PDE approach and by means of the tools of the control theory.

5.3.5. Optimal control of first order HJ equations with linearly bounded Hamiltonian

Participant: Philip Graber.

In [40], we consider the optimal control of solutions of first order Hamilton-Jacobi equations, where the Hamiltonian is convex with linear growth. This models the problem of steering the propagation of a front by constructing an obstacle. We prove existence of minimizers to this optimization problem as in a relaxed setting and characterize the minimizers as weak solutions to a mean field game type system of coupled partial differential equations. Furthermore, we prove existence and partial uniqueness of weak solutions to the PDE system. An interpretation in terms of mean field games is also discussed.

5.3.6. Zubov's equation for state-constrained perturbed nonlinear systems

Participant: Hasnaa Zidani.

The paper [41] gives a characterization of the uniform robust domain of attraction for a nite non-linear controlled system subject to perturbations and state constraints. We extend the Zubov approach to characterize this domain by means of the value function of a suitable in nite horizon state-constrained control problem which at the same time is a Lyapunov function for the system. We provide associated Hamilton-Jacobi-Bellman equations and prove existence and uniqueness of the solutions of these generalized Zubov equations.

5.3.7. Numerical methods for chance-constrained stochastic optimal control problems

Participant: Laurent Pfeiffer.

In Laurent Pfeiffer's PhD, we study stochastic optimal control problems with a probability constraint on the final state. This constraint must be satisfied with a probability greater or equal than a given level. We analyse and compare two approaches for discrete-time problems: a first one based on a dynamic programming principle and a second one using Lagrange relaxation. These approaches can be used for continuous-time problems, for which we give numerical illustrations.

CORIDA Project-Team

5. New Results

5.1. Analysis and control of fluids and of fluid-structure interactions

In [47], we analyze the system fluid-rigid body in the case of where the rigid body is a ball of "small radius". More precisely, we consider the limit system as the radius goes to zero. We recover the Navier-Stokes system with a particle following the the velocity of the fluid. We consider in [45] a model of vesicle moving into a viscous incompressible fluid. Such a model, based on a phase-field approach was derived by researchers in Physics, and is quite difficult to study. By considering some approximation, we prove some result of existence of solutions for such a system.

By acting on a part of the fluid domain or on a part of the exterior boundary, we aim at controlling the fluid velocity, the rigid velocity and the position of the rigid body. It can be a control in open loop or in closed loop. We have studied both problems in the 1D case. In this case, the study benefits some simplifications, but can also be more difficult since the fluid domain is no more connected. As a consequence, if one wants to control by using only one input, on one part of the fluid domain, the fluid on the other side of the particle is only controlled by the motion of the structure.

We introduce a new method for controllability of nonlinear parabolic system allowing to deal with this problem and we solve it in ([24]). We also obtain the local stabilization of such system around a stationary state in [41].

We study the Cauchy problem corresponding to a similar 1D system without viscosity in [40]. In that case, we have to deal with the interaction between the particle and shock waves or relaxation waves. In [44], we analyze a numerical scheme for the method of observers used to reconstruct the initial data of hyperbolic systems such as wave equation. We add some numerical viscosity in the scheme in order to have a uniform decay of the error between the reconstructed solution and the real one.

In [30], a Lagrange-Galerkin method is introduced to approximate a two dimensional fluid-structure interaction problem for deformable solids. The new numerical scheme we present is based on a characteristics function mapping the approximate deformable body at the discrete time level t_{k+1} into the approximate body at time t_k.

The aim of [25] is to tackle the time optimal controllability of an $(n+1)$-dimensional nonholonomic integrator with state constraints. A full description of an optimal control together with the corresponding optimal trajectories are explicitly obtained. The optimal trajectories we construct, are composed of arcs of circle lying in a 2-dimensional plane.

In [26], controllability results are obtained for a low Reynolds number swimmer composed by a spherical object which is undergoing radial and axi-symmetric deformations in order to propel itself in a viscous fluid governed by the Stokes equations. A time optimal control problem is also solved for a simplified model and explicit optimal solutions are constructed.

5.2. Frequency domain methods for the analysis and control of systems governed by PDE's

With a numerical viscosity terms in the approximation scheme of second order evolution equations, we show in [11] the exponential or polynomial decay of the discrete scheme when the continuous problem has such a decay and when the spectrum of the spatial operator associated with the undamped problem satisfies the generalized gap condition. We further show the convergence of the discrete solution to the continuous one.

In [19], we propose a strategy to determine the Dirichlet-to-Neumann (DtN) operator for infinite, lossy and locally perturbed hexagonal periodic media, using a factorization of this operator involving two non local operators. The first one is a DtN type operator and corresponds to a half-space problem, while the second one is a Dirichlet-to-Dirichlet (DtD) type operator related to the symmetry properties of the problem.

In [22], we generalize to the case of acoustic penetrable scatterers the results derived by Hazard and Ramdani [54] for sound hard scatterers. In particular, we provide a justification of the DORT method in this case and we show that each small inhomogeneity gives rise to $3d + 1$ eigenvalues of the time reversal operator. The selective focusing of the corresponding eigenfunctions is also proved.

In [17], we consider the inverse problem of determining the potential in the dynamical Schrödinger equation on the interval by the measurement on the boundary. We use the Boundary Control Method to recover the spectrum of the problem from the observation at either left or right end points. Using the specificity of the one-dimensional situation we recover the spectral function, reducing the problem to the classical one which could be treated by known methods. We also consider the case where only a finite number (N) of eigenvalues are available and we prove the convergence of the reconstruction method as N tends to infinity.

We give some spectral and condition number estimates of the acoustic single-layer operator for low-frequency multiple scattering in dense [15] and dilute [16] media.

5.3. Use of geometric techniques for the control of finite and infinite dimensional systems

The paper [31] deals with the design of high gain observers for a class of continuous dynamical systems with discrete-time measurements. The new idea of the this work is to synthesize an observer requiring the less knowledge as possible from the output measurements. This is done by using an updated sampling time observer.

In [12], it is shown that, for a bilinear system, the property of observability is preserved after sampling provided that the controls take their values in a compact space and do not vary too quickly.

In the note [18] two notions of controllability are studied, called respectively radial controllability and directional controllability. It is proven that for families of linear vector fields, the two notions are actually equivalent.

We used operators theory to obtain some new estimates of the energy of an infinite dimensional bilinear quantum systems. These results were presented in [34].

Robust control of bilinear Schrödinger equation was investigated in [35]. The use of sharp finite dimensional energy estimates (in the spirit of [34]) allows to obtain the first approximate ensemble controllability results for infinite dimensional quantum systems, also in presence of mixed spectrum for the free Hamiltonian.

The above energy questions, together with a their relation with some open question in the control of bilinear quantum systems, were gathered in the survey [32].

Our team is heavily involved in the optimization of driving strategy, and especially in the effective implementation in the prototype build in ESSTIN. MPC related methods have been tested and successfully improved as described in [37].

DISCO Project-Team

6. New Results

6.1. Equidimensional block-triangular representation of linear functional systems

Participant: Alban Quadrat.

In [30], it is shown that every linear functional system (e.g., PD systems, differential time-delay systems, difference systems) is equivalent to a linear functional system defined by an upper block-triangular matrix of functional operators: each diagonal block is respectively formed by a generating set of the elements of the system satisfying a purely i-codimensional system. Hence, the system can be integrated in cascade by successively solving (inhomogeneous) i-codimensional linear functional systems to get a Monge parametrization of its solution space [120]. The results are based on an explicit construction of the grade/purity filtration of the module associated with the linear functional system. This new approach does not use complex Grothendieck spectral sequence arguments as is done in the literature of modern algebra [86], [87]. To our knowledge, the algorithm obtained in [30] is the most efficient algorithm existing in the literature of non-commutative algebra. It was implemented in the PURITYFILTRATION package developed in Maple (see Section 5.6) and in the `homalg` package of GAP 4 (see Section 5.7). Classes of overdetermined/underdetermined linear systems of partial differential equations which cannot be directly integrated by Maple can be solved using the PURITYFILTRATION package.

6.2. Serre's reduction of linear functional systems and related problems

Participants: Alban Quadrat, Thomas Cluzeau [ENSIL, Univ. Limoges].

Given a linear multidimensional system (e.g., ordinary/partial differential systems, differential time-delay systems, difference systems), Serre's reduction aims at finding an equivalent linear multidimensional system which contains fewer equations and fewer unknowns. Finding Serre's reduction of a linear multidimensional system can generally simplify the study of structural properties and of different numerical analysis issues, and it can sometimes help solving the linear multidimensional system in closed form. The connection between Serre's reduction and the decomposition problem [94], which aims at finding an equivalent linear functional system which is defined by a block diagonal matrix of functional operators, is algorithmically studied in [41], [42]. Moreover, a characterization of isomorphic finitely presented modules in terms of certain inflations of their presentation matrices is obtained in [42]. This result yields a connection between a certain matrix completion problem and Serre's reduction [42].

6.3. Algorithmic study of linear PD systems and Stafford's theorems

Participants: Alban Quadrat, Daniel Robertz [Univ. Aachen].

In [121],[82], algorithmic versions of Stafford's results [124] (e.g., computation of unimodular elements, decomposition of modules, Serre's splitting-off theorem, Stafford's reduction, Bass' cancellation theorem, minimal number of generators) were obtained and implemented in the STAFFORD package [82]. In particular, we show how a determined/overdetermined linear system of partial differential equations with either polynomial, rational, formal power series or locally convergent power series coefficients is equivalent to a linear system of partial differential equations with at most two unknowns. This result is a large generalization of the cyclic vector theorem which plays an important role in the theory of linear ordinary differential equations.

6.4. Foundations of the behavioural approach

Participant: Alban Quadrat.

Within the algebraic analysis approach to behaviours [91], [113], in [34], we propose to consider a system not only as a behaviour $\mathrm{ext}^0_D(M,\mathcal{F})$ [107], where M is the finitely presented left D-module defined by the matrix defining the system and $\mathcal{F}$ the signal space, but as the set of all the $\mathrm{ext}^i_D(M,\mathcal{F})$'s, where $0 \leq i \leq n$, where n is the global dimension of D. In this new framework, using Yoneda product, the left D-homomorphims of M [94] and the internal symmetries of the behaviour $\mathrm{ext}^0_D(M,\mathcal{F})$ [94] are generalized to the full system $\{\mathrm{ext}^i_D(M,\mathcal{F})\}_{i=0,\ldots,n}$ In particular, a system-theoretic interpretation of the Yoneda product is given.

In [117], we study the construction of a double complex leading to a Grothendieck spectral sequence converging to the obstructions $\mathrm{tor}^i_D(N,\mathcal{F})$'s for the existence of a chain of successive parametrizations starting with the behaviour $\mathrm{ext}^0_D(M,\mathcal{F})$, where N is the Auslander transpose of M. These obstructions $\mathrm{tor}^i_D(N,\mathcal{F})$ can be studied by means of a long process starting with the $\mathcal{F}$-obstructions $\mathrm{ext}^j_D(\mathrm{ext}^k_D(N,D),\mathcal{F})$'s for the solvability of certain inhomogeneous linear systems defined by the algebraic obstructions $\mathrm{ext}^k_D(N,D)$'s measuring how far M is for being a projective left D-module. Hence, the algebraic properties of the left D-module M, defining the behaviour $\mathrm{ext}^0_D(M,\mathcal{F})$, and the functional properties of the signal space $\mathcal{F}$ can be simultaneously used to study the obstructions for the existence of a chain of successive parametrizations starting with the behaviour $\mathrm{ext}^0_D(M,\mathcal{F})$. These results can be used to find again the different situations studied in the literature (e.g., cases of an injective or a flat left D-module $\mathcal{F}$). Finally, setting $\mathcal{F} = D$, the above results can be used to find again the characterization of the grade/purity filtration of M by means of a Grothendieck spectral sequence. See Section 6.1 and [86], [87], [30].

Within the algebraic analysis approach to behaviours [91], [113], in [116], we explain how the concept of inverse image of a finitely presented left D-module M, defining the behaviour $\mathrm{ext}^0_D(M,\mathcal{F})$ [107], can be used to study the problem of characterizing the restriction of the behaviour $\mathrm{ext}^0_D(M,\mathcal{F})$ to a non characteristic submanifold of $\mathbb{R}^n$. In particular, we detail the explict construction of inverse images of left D-modules for standard maps.

6.5. Boundary value problems for linear ordinary integro-differential equations

Participants: Alban Quadrat, Georg Regensburger.

In [35], we study algorithmic aspects of linear ordinary integro-differential operators with polynomial coefficients. Even though this algebra is not noetherian and has zero divisors, Bavula recently proved in [85] that it is coherent, which allows one to develop an algebraic systems theory. For an algorithmic approach to linear systems theory of integro-differential equations with boundary conditions, computing the kernel of matrices is a fundamental task. As a first step, we have to find annihilators, which is, in turn, related to polynomial solutions. We present an algorithmic approach for computing polynomial solutions and the index for a class of linear operators including integro-differential operators. A generating set for right annihilators can be constructed in terms of such polynomial solutions. For initial value problems, an involution of the algebra of integro-differential operators also allows us to compute left annihilators, which can be interpreted as compatibility conditions of integro-differential equations with boundary conditions. These results are implemented in MAPLE based on the `IntDiffOp` and `IntDiffOperations` packages.

6.6. Noncommutative geometry approach to infinite-dimensional systems

Participant: Alban Quadrat.

In [112], [111], [110], it was shown how the fractional representation approach to analysis and synthesis problems developed by Vidyasagar, Desoer, Callier, Francis, Zames..., could be recast into a modern algebraic analysis approach based on module theory (e.g., fractional ideals, algebraic lattices) and the theory of Banach algebras. This new approach successfully solved open questions in the literature. Basing ourselves on this new approach, we explain in [114], [115] why the non-commutative geometry developed by Alain Connes is a natural framework for the study of stabilizing problems of infinite-dimensional systems. Using the 1-dimensional quantized calculus developed in non-commutative geometry and results obtained in [112], [111], [110], we show that every stabilizable system and their stabilizing controllers naturally admit geometric

structures such as connections, curvatures, Chern classes, ... These results developed in [114], [115] are the first steps toward the use of the natural geometry of the stabilizable systems and their stabilizing controllers in the study of the important H_∞ and H_2-problems.

6.7. Stability analysis of fractional neutral systems with commensurate delays

Participants: Le Ha Vy Nguyen, Catherine Bonnet.

Fractional neutral systems with commensurate delays have chains of poles aymptotic to vertical lines. The case where the imaginary axis is an asymptotic one is interesting. Indeed, if the system has some chains of poles asymptotic to the imaginary axis, then the fact that all poles lie in the open left half-plane does not guarantee the H_∞-stability of the system.

This kind of systems was studied in [97], [104]. In [97], systems with single chains of poles asymptotic to the imaginary axis was considered and necessary and sufficient conditions for H_∞-stability were derived. Some particular systems with multiple chains have been examined in [104]. We have extended this year this study to more general systems with multiple chains of poles approaching the imaginary axis.

6.8. Stabilization of fractional neutral systems with commensurate delays

Participants: Le Ha Vy Nguyen, Catherine Bonnet.

We consider fractional neutral systems with commensurate delays which may have chains of poles asymptotic to vertical lines lying in the open left half-plane and have chains clustering the imaginary axis. Due to the latter, the system may possess infinitely many poles in the right half-plane. We prove that a class of rational fractional controllers cannot stabilize this kind of systems in the sense of H_∞ except in a simple case. For this case, thanks to the fractional PI controller given in [1], a parametrization of stabilizing controllers is derived [105].

6.9. Stabilization of MISO fractional systems with delays

Participants: Le Ha Vy Nguyen, Catherine Bonnet.

In order to yield the set of all the stabilizing controllers of a class of MISO fractional systems with delays by mean of Youla-Kucera parametrization regarding H_∞-stability, we are interested in determining coprime factorizations of the transfer function. Explicit expressions of left coprime factorizations and left Bézout factors have been derived in [103]. We have continued this year to search for explicit expressions of right coprime factorizations for some classes of systems [63].

6.10. Interval Observer

Participants: Frédéric Mazenc [correspondent], Thach Ngoc Dinh, Silviu Iulian Niculescu.

We made several progresses in the domain of the construction of state estimators called interval observers.

1) In [18], we have shown how interval observers can be constructed for nonlinear (and not Lipschitz) systems possessing a special triangular system.

2) The contributions [20] and [55] present a new major result for the design of interval observers for discete-time systems with input and output: it is explained how two classical Luenberger obsevers can be used, even in the absence of the positivity property as interval observer, provided two appropriate output, which compose the lower and the upper bound of the interval observer, are selected. In [19], coordinate transformations which change an arbitrary linear discrete-time system into a positive one and general nonlinear design of interval observers for nonlinear systems (satisfying a restricitive stability assumption) are proposed.

3) The paper [54] presents the first construction of continuous-discrete interval observer for linear continuous-time systems with discrete measurements. The importance in engineering applications of this result is clear: most of the time the measured variables are available at discrete instants only. The result relies on the design of changes of coordinates which transform a linear system into a nonnegative one, but the dynamic part of interval observers is not cooperative.

6.11. Reduction model approach: new advances

Participants: Frédéric Mazenc [correspondent], Michael Malisoff [Louisiana State University], Silviu Iulian Niculescu, Dorothé Normand-Cyrot [L2S, CNRS].

We solved several distinct problems entailing to the celebrated reduction model approach. Let us recall that this technique makes it possible to stabilize systems with arbitrarily large pointwise or distributed delay in the input.

1) We proposed in [25] a new construction of exponentially stabilizing sampled feedbacks for continuous-time linear time-invariant systems with an arbitrarily large constant pointwise delay in the inputs. Stability is guaranteed under an assumption on the size of the largest sampling interval. The proposed design is based on an adaptation of the reduction model approach. The stability of the closed loop systems is proved through a Lyapunov-Krasovskii functional of a new type, from which is derived a robustness result

2) The paper [59] presents several results pertaining to the stabilization with feedbacks given by an explicit formula of linear time varying systems in the case where there is a constant delay in the input. In addition, it establishes input-to-state stability with respect to additive uncertainties. As a particular case, we considered a large class of rapidly time varying systems and provided a lower bound on the admissible rapidness parameters. We illustrated our results using a pendulum model.

3) The paper [24], which is devoted to the original problem of stabilizing nonlinear systems with input with distributed delay, is actually not an extension of the reduction model approach, but it complements it and uses operators which have been inspired by those used in the classical context of the reduction model theory.

6.12. Neutral systems and integral equations

Participants: Frédéric Mazenc [correspondent], Hiroshi Ito [Kyushu Institute of Technology], Pierdomenico Pepe [Univ. of L'Aquila].

1) For nonlinear systems with delay of neutral type, we developped a new technique of stability and robustness analysis. It relies on the construction of functionals which make it possible to establish estimates of the solutions different from, but very similar to, estimates of ISS or iISS type. These functionals are themselves different from, but very similar to, ISS or iISS Lyapunov-Krasovskii functionals. The approach applies to systems which do not have a globally Lipschitz vector field and are not necessarily locally exponentially stable. We apply this technique to carry out a backstepping design of stabilizing control laws for a family of neutral nonlinear systems [21].

2) In a second paper [57], we extended the previous results to the problem of deriving stability and stabilizability conditions for nonlinear systems with delay interconnected with an integral equation via the construction of a Lyapunov-Krasovskii functional.

6.13. Nonlinear systems with delay

Participants: Frédéric Mazenc [correspondent], Michael Malisoff [Louisiana State University], Thach Ngoc Dinh.

We obtained new results on the robustness analysis of nonlinear systems belonging to a general family when they are globally stabilized by a state feedback corrupted by the presence of a delay and sampling [22], [58]. The result is based on the construction of a non-quadratic Lyapunov-Krasovskii functional.

In [23], a problem of state feedback stabilization of time-varying feedforward systems with a pointwise delay in the input is solved. The approach we adopted relies on a time-varying change of coordinates and Lyapunov-Krasovskii functionals. The result applies for any given constant delay, and provides uniformly globally asymptotically stabilizing controllers of arbitrarily small amplitude. The closed-loop systems enjoy input-to-state stability properties with respect to additive uncertainty on the controllers. The work was illustrated through a tracking problem for a model for high level formation flight of unmanned air vehicles.

6.14. Set theoretic fault detection and isolation

Participant: Sorin Olaru.

Fault-tolerant control theory is a well-studied topic but the use of the sets in detection, isolation and/or reconfiguration is rather tangential. Sorin Olaru together with his collaborators (and principally with F. Stoican) conducted a systematic analysis of the set-theoretic elements and devise approaches which exploit advanced elements within the field. The main idea is to translate fault detection and isolation conditions into those conditions involving sets. Furthermore, these are to be computed efficiently using positive invariance and reachability notions. Constraints imposed by exact fault control are used to define feasible references (which impose persistent excitation and, thus, non-convex feasible sets). Particular attention is given to the reciprocal influences between fault detection and isolation on the one hand, and control reconfiguration on the other. The recent results on this topic are gathered in the recent book [81].

A new result has been obtained by the use of controlled invariance for the separation of faulty/healthy invariant sets in the detection and isolation [32] based on the necessary and sufficent conditions of George Bitsoris.

In a series of recent papers [67], [68], [70], [69], the link between the interval observers and the invariant sets have been investigated by establishing a series of formal results on the limit behaviour with potential applications in the detection and isolation of actuators faults

6.15. Model Predictive Control: distributed formulations and collision avoidance problems

Participant: Sorin Olaru.

In [78], the mixt integer techniques have been analysed in the distributed model predictive control context, underlining the dependence of collision avoidance mechanism on the obstacle modeling and susequently on their treatement inside optimization-based control techniques as MPC (model predictive control). On the same topic of adversary consraints, a geometrical conditions has been establised in [71] for the local stabilization of a linear dynamics on a boundary of a forbidden region in the state space.

The theoretical developments from the last two years on the MPC design for multi-agent control problem led to the succesful application of receding horizon flight control for trajectory tracking of autonomous aerial vehicles [28]. In the same line or research, the predictive control for trajectory tracking and decentralized navigation of multi-agent formations has been presented in [29].

In [66] a Characterization of the Relative Positioning of Mobile Agents for Full Sensorial Coverage in an Augmented Space with Obstacles is presented in view of a MPC control design.

A predictive control-based algorithm for path following of autonomous aerial vehicles has been proposed in [65] to improve the previous trajectory tracking mechanism. The ultimate goal oof both schemes is to avoid the real-time infeasibility problems in MPC.

The distributed predictive control mechanisms have been used for the control of a four interconnected tanks benchmark [48], proving the versatility of a nonlinear Distributed MPC technique previously proposed by A. Grancharova.

In [62] the distributed Model Predictive Control of Leader-Follower Systems has been studied using an interior point method with efficient computations leading to simple tuning mechanisms for the cost functions and the terminal sets of the local MPC sub-problems.

6.16. Invariant sets in control

Participant: Sorin Olaru.

The longstanding research interest on the positive invaraince of a set with respect to the trajectories of the dynamical systems allowed recently the statement of explicit invariant approximation of the maximal robust positive invariant ser for LTI dynamics with zonotopic disturbances [51].

In the class of hybrid dynamical systems, explicit robustness and fragility margins for discrete-time linear systems with PWA control has been established in [64] by means of positive invariance arguments.

In [37] a series of new results on the linear constrained regulation problem have been presented by completing the classical results with the case of active constraints for the equilibrium point.

6.17. Optimization of mu-analysis parameterization

Participant: Guillaume Sandou [correspondent].

The robustness against parametric uncertainties can be studied using the structured singular value mu. In that case, a normalization of the uncertain parameters is performed, and the mu analysis provides the larger parallelepiped centered in the nominal and included in the stability domain. However, results depend on the initial normalization. In this study, the normalization is optimized so as to get the largest guaranteed stability domain. The corresponding problem being highly nonlinear, a metaheuristic method, Particle Swarm Optimization, is used for that purpose. An academic and a real life example, namely the pendulum in the cart problem, have been used to prove the viability of the approach.

6.18. Optimal weight tuning in Hinfinity loop-shaping with PSO considering time constraints

Participants: Guillaume Sandou [correspondent], Gilles Duc [Supélec, E3S], Philippe Feyel [Sagem].

Hinfinity loop-shaping controllers have proven their efficiency to solve problems based on complex industrial specifications. However, the tuning of the weighting filters is a time consuming task. This work deals with the use of metaheuristics optimization for this weighting filter tuning. Whereas this topic has already been investigated in lot of works, all of them assume a particular pole/zero/damping/pulse expression for the searched transfer function. But choosing the best weight structure is not trivial and may lead to suboptimal solutions for the design process. That is why, we propose to enhance the weight selection problem by relaxing the structure constraints of transfer functions. The developed methodology is tested, using a real industrial example and leads to satisfactory results.

6.19. mu-synthesis with dynamic D-Scalings using Quantum Particle Swarm Optimization

Participants: Guillaume Sandou [correspondent], Gilles Duc [Supélec, E3S], Philippe Feyel [Sagem].

This study proposes to revisit the mu-synthesis problem with a recent and efficient meta-heuristic called Quantum Particle Swarm Optimization (QPSO). This algorithm allows us to optimizing dynamics (or static) D-scalings without fitting them which leads to robust performance controllers. This method has been applied to an industrial problem and has been proven to be better than the classical D-K iteration method.

6.20. Stabilization of time-delay systems

Participants: Alban Quadrat, Arnaud Quadrat [SAGEM, MASSY].

In [118], [122], we study the stabilization problem of a linear system formed by a simple integrator and a time-delay system. We show that the stabilizing controllers of such a system can be rewritten as the closed-loop system defined by the stabilizing controllers of the simple integrator and a distributed delay system. This result is used to study tracking problems appearing in the study of inertially stabilized platforms for optical imaging systems. Moreover, an elementary proof for the parametrization [111] of all stabilizing controllers of a stabilizable plant − which does not necessarily admits doubly coprime factorizations − is given in [122].

6.21. A Stabilization problem in chemostats

Participants: Frédéric Mazenc [correspondent], Jérôme Harmand [LBE INRA, EPI MODEMIC].

We have considered the classical model of the chemostat (which is a bio-reactor) with one substrate, one species and a Haldane type growth rate function is considered. The input substrate concentration is supposed to be constant and the dilution rate is considered as the control. The problem of globally asymptotically stabilizing a positive equilibrium point of this system in the case where the measured concentrations are delayed and piecewise constant with a piecewise constant control is addressed. The result relies on the introduction of a dynamic extension of a new type. [56].

6.22. Control design for UAVs

Participants: Frédéric Mazenc [correspondent], Michael Malisoff [Louisiana State University].

In [14], we studied a kinematic model that is suitable for control design for high level formation flight of UAVs (Unmanned Aerial Vehicles). We designed controllers that give robust global tracking for a wide class of reference trajectories in the sense of the robustness notion called input-to-state stability. The control laws satisfy amplitude and rate constraints.

6.23. Modeling and control of Acute Myeloid Leukemia

Participants: José Luis Avila Alonso [correspondent], Annabelle Ballesta [BANG project-team], Frédéric Bonnans [COMMANDS project-team], Catherine Bonnet, Jean Clairambault [BANG project-team], Xavier Dupuis [COMMANDS project-team], Pierre Hirsch [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Jean-Pierre Marie [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Faten Merhi [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris], Silviu Iulian Niculescu, Hitay Özbay [Bilkent University, Ankara, Turkey], Ruoping Tang [INSERM Paris (Team18 of UMR 872) Cordeliers Research Centre and St. Antoine Hospital, Paris].

In [75] we propose a new mathematical model of the cell dynamics in Acute Myeloid Leukemia (AML) which takes into account the four different phases of the proliferating compartment. The dynamics of the cell populations are governed by transport partial differential equations structured in age and by using the method of characteristics, we obtain that the dynamical system of equation can be reduced to two coupled nonlinear equations with four internal sub-systems involving distributed delays. Local stability conditions for a particular equilibrium point, corresponding to a positive cells, are derived in terms of a set of inequalities involving the parameters of the mathematical model. A parameter estimation of our model is being performed using biological data (Annabelle Ballesta).

We have also studied a coupled model for healthy and cancer cell dynamics in Acute Myeloid Leukemia consisting of two stages of maturation for cancer cells and three stages of maturation for healthy cells. The cell dynamics are modelled by nonlinear partial differential equations. The interconnection phenomenon between the healthy and cancer cells takes place on the re-introduction functions leaving the resting compartments to the proliferating compartments of both populations of cells at the first stage. For a particular healthy equilibrium point, locally stability conditions involving the parameters of the mathematical model are obtained [83], [84].

GECO Project-Team

6. New Results

6.1. New results: geometric control

We start by presenting some results on motion planning and tracking algorithms.

- In [22] we study the complexity of the motion planning problem for control-affine systems. Such complexities are already defined and rather well-understood in the particular case of nonholonomic (or sub-Riemannian) systems. Our aim is to generalize these notions and results to systems with a drift. Accordingly, we present various definitions of complexity, as functions of the curve that is approximated, and of the precision of the approximation. Due to the lack of time-rescaling invariance of these systems, we consider geometric and parametrized curves separately. Then, we give some asymptotic estimates for these quantities.
- In [23] we study the problem of controlling an unmanned aerial vehicle (UAV) to provide a target supervision and to provide convoy protection to ground vehicles. We first present a control strategy based upon a Lyapunov–LaSalle stabilization method to provide supervision of a stationary target. The UAV is expected to join a pre-designed admissible circular trajectory around the target which is itself a fixed point in the space. Our strategy is presented for both HALE (High Altitude Long Endurance) and MALE (Medium Altitude Long Endurance) types UAVs. A UAV flying at a constant altitude (HALE type) is modeled as a Dubins vehicle (i.e. a planar vehicle with constrained turning radius and constant forward velocity). For a UAV that might change its altitude (MALE type), we use the general kinematic model of a rigid body evolving in $\mathbb{R}^3$. Both control strategies presented are smooth and unlike what is usually proposed in the literature these strategies asymptotically track a circular trajectory of exact minimum turning radius. We then consider the problem of adding to the tracking task an optimality criterion. In particular, we present the time-optimal control synthesis for tracking a circle by a Dubins vehicle. This optimal strategy, although much simpler than the point-to-point time-optimal strategy obtained by P. Souéres and J.-P. Laumond in the 1990s, is very rich. Finally, we propose control strategies to provide supervision of a moving target, that are based upon the previous ones.
- In [26] we prove the continuity and the Hölder equivalence w.r.t. an Euclidean distance of the value function associated with the L^1 cost of the control-affine system $\dot{q} = f_0(q) + \sum_{j=1}^{m} u_j f_j(q)$, satisfying the strong Hörmander condition. This is done by proving a result in the same spirit as the Ball-Box theorem for driftless (or sub-Riemannian) systems. The techniques used are based on a reduction of the control-affine system to a linear but time-dependent one, for which we are able to define a generalization of the nilpotent approximation and through which we derive estimates for the shape of the reachable sets. Finally, we also prove the continuity of the value function associated with the L^1 cost of time-dependent systems of the form $\dot{q} = \sum_{j=1}^{m} u_j f_j^t(q)$.

Let us list some new results in sub-Riemannian geometry and hypoelliptic diffusion.

- In [1] we provide normal forms for 2D almost-Riemannian structures, which are generalized Riemannian structures on surfaces for which a local orthonormal frame is given by a Lie bracket generating pair of vector fields that can become collinear. Generically, there are three types of points: Riemannian points where the two vector fields are linearly independent, Grushin points where the two vector fields are collinear but their Lie bracket is not, and tangency points where the two vector fields and their Lie bracket are collinear and the missing direction is obtained with one more bracket. We consider the problem of finding normal forms and functional invariants at each type of point. We also require that functional invariants are “complete” in the sense that they permit to recognize locally isometric structures. The problem happens to be equivalent to the one of finding a smooth canonical parameterized curve passing through the point and being transversal to the distribution.

For Riemannian points such that the gradient of the Gaussian curvature K is different from zero, we use the level set of K as support of the parameterized curve. For Riemannian points such that the gradient of the curvature vanishes (and under additional generic conditions), we use a curve which is found by looking for crests and valleys of the curvature. For Grushin points we use the set where the vector fields are parallel. Tangency points are the most complicated to deal with. The cut locus from the tangency point is not a good candidate as canonical parameterized curve since it is known to be non-smooth. Thus, we analyze the cut locus from the singular set and we prove that it is not smooth either. A good candidate appears to be a curve which is found by looking for crests and valleys of the Gaussian curvature. We prove that the support of such a curve is uniquely determined and has a canonical parametrization.

- The curvature discussed in [14] is a rather far going generalization of the Riemann sectional curvature. We define it for a wide class of optimal control problems: a unified framework including geometric structures such as Riemannian, sub-Riemannian, Finsler and sub-Finsler structures; a special attention is paid to the sub-Riemannian (or Carnot–Caratheodory) metric spaces. Our construction of the curvature is direct and naive, and it is similar to the original approach of Riemann. Surprisingly, it works in a very general setting and, in particular, for all sub-Riemannian spaces.
- In [15] we provide the small-time heat kernel asymptotics at the cut locus in three relevant cases: generic low-dimensional Riemannian manifolds, generic 3D contact sub-Riemannian manifolds (close to the starting point) and generic 4D quasi-contact sub-Riemannian manifolds (close to a generic starting point). As a byproduct, we show that, for generic low-dimensional Riemannian manifolds, the only singularities of the exponential map, as a Lagragian map, that can arise along a minimizing geodesic are A_3 and A_5 (in the classification of Arnol'd's school). We show that in the non-generic case, a cornucopia of asymptotics can occur, even for Riemannian surfaces.
- In [19] we study the evolution of the heat and of a free quantum particle (described by the Schroedinger equation) on two-dimensional manifolds endowed with the degenerate Riemannian metric $ds^2 = dx^2 + |x|^{-2\alpha} d\theta^2$, where $x \in \mathbb{R}$, $\theta \in \mathbb{T}$ and the parameter $\alpha \in \mathbb{R}$. For $\alpha \leq -1$ this metric describes cone-like manifolds (for $\alpha = -1$ it is a flat cone). For $\alpha = 0$ it is a cylinder. For $\alpha \geq 1$ it is a Grushin-like metric. We show that the Laplace–Beltrami operator Δ is essentially self-adjoint if and only if $\alpha \notin (-3, 1)$. In this case the only self-adjoint extension is the Friedrichs extension Δ_F, that does not allow communication through the singular set $\{x = 0\}$ both for the heat and for a quantum particle. For $\alpha \in (-3, -1]$ we show that for the Schroedinger equation only the average on θ of the wave function can cross the singular set, while the solutions of the only Markovian extension of the heat equation (which indeed is Δ_F) cannot. For $\alpha \in (-1, 1)$ we prove that there exists a canonical self-adjoint extension Δ_B, called bridging extension, which is Markovian and allows the complete communication through the singularity (both of the heat and of a quantum particle). Also, we study the stochastic completeness (i.e., conservation of the L^1 norm for the heat equation) of the Markovian extensions Δ_F and Δ_B, proving that Δ_F is stochastically complete at the singularity if and only if $\alpha \leq -1$, while Δ_B is always stochastically complete at the singularity.

6.2. New results: quantum control

New results have been obtained for the control of the bilinear Schrödinger equation.

- In [4] we show the approximate rotational controllability of a polar linear molecule by means of three nonresonant linear polarized laser fields. The result is based on a general approximate controllability result for the bilinear Schroedinger equation, with wavefunction varying in the unit sphere of an infinite-dimensional Hilbert space and with several control potentials, under the assumption that the internal Hamiltonian has discrete spectrum. A further general results, extending the above approach, are obtained in [16].
- In [5] we provide a short introduction to modern issues in the control of infinite dimensional closed quantum systems, driven by the bilinear Schroedinger equation. The first part is a quick presentation

of some of the numerous recent developments in the fields. This short summary is intended to demonstrate the variety of tools and approaches used by various teams in the last decade. In a second part, we present four examples of bilinear closed quantum systems. These examples were extensively studied and may be used as a convenient and efficient test bench for new conjectures. Finally, we list some open questions, both of theoretical and practical interest.

- In [6] we study the so-called spin-boson system, namely a spin-1/2 particle in interaction with a distinguished mode of a quantized bosonic field. We control the system via an external field acting on the bosonic part. Applying geometric control techniques to the Galerkin approximation and using perturbation theory to guarantee non-resonance of the spectrum of the drift operator, we prove approximate controllability of the system, for almost every value of the interaction parameter.
- In [9] and [25] we investigate the controllability of a quantum electron trapped in a two-dimensional device. The problem is modeled by the Schroedinger equation in a bounded domain coupled to the Poisson equation for the electrical potential. The controller acts on the system through the boundary condition on the potential, on a part of the boundary modeling the gate. We prove that, generically with respect to the shape and boundary conditions on the gate, the device is controllable. In [25] We also consider control properties of a more realistic nonlinear version of the device, taking into account the self-consistent electrostatic Poisson potential.
- In [18] we study the controllability of a closed control-affine quantum system driven by two or more external fields. We provide a sufficient condition for controllability in terms of existence of conical intersections between eigenvalues of the Hamiltonian in dependence of the controls seen as parameters. Such spectral condition is structurally stable in the case of three controls or in the case of two controls when the Hamiltonian is real. The spectral condition appears naturally in the adiabatic control framework and yields approximate controllability in the infinite-dimensional case. In the finite-dimensional case it implies that the system is Lie-bracket generating when lifted to the group of unitary transformations, and in particular that it is exactly controllable. Hence, Lie algebraic conditions are deduced from purely spectral properties. Another contribution of [18] is the proof that approximate and exact controllability are equivalent properties for general finite-dimensional quantum systems.

6.3. New results: neurophysiology

- In recent papers models of the human locomotion by means of an optimal control problem have been proposed. In this paradigm, the trajectories are assumed to be solutions of an optimal control problem whose cost has to be determined. The purpose of [3] is to analyze the class of optimal control problems defined in this way. We prove strong convergence result for their solutions on the one hand for perturbations of the initial and final points (stability), and on the other hand for perturbations of the cost (robustness).
- [8] analyses a class of optimal control problems on geometric paths of the euclidean space, that is, curves parametrized by arc length. In the first part we deal with existence and robustness issues for such problems and we define the associated inverse optimal control problem. In the second part we discuss the inverse optimal control problem in the special case of planar trajectories and under additional assumptions. More precisely we define a criterion to restrict the study to a convenient class of costs based on the analysis of experimentally recorded trajectories. This method applies in particular to the case of human locomotion trajectories.
- The article [17] presents an algorithm implementing the theory of neurogeometry of vision, described by Jean Petitot in his book. We propose a new ingredient, namely working on the group of translations and discrete rotations $\mathrm{SE}(2, N)$. We focus on the theoretical and numerical aspects of integration of an hypoelliptic diffusion equation on this group. Our main tool is the generalized Fourier transform. We provide a complete numerical algorithm, fully parallellizable.

6.4. New results: switched systems

- In [2] we study the control system $\dot{x} = Ax + \alpha(t)bu$ where the pair (A, b) is controllable, $x \in \mathbb{R}^2$, $u \in \mathbb{R}$ is a scalar control and the unknown signal $\alpha : \mathbb{R}_+ \to [0, 1]$ is (T, μ)-persistently exciting (PE), i.e., there exists $T \geq \mu > 0$ such that, for all $t \in \mathbb{R}_+$, $\int_t^{t+T} \alpha(s)ds \geq \mu$. We are interested in the stabilization problem of this system by a linear state feedback $u = -Kx$. In [2], we positively answer a question asked in [52] and prove the following: Assume that the class of (T, μ)-PE signals is restricted to those which are M-Lipschitzian, where $M > 0$ is a positive constant. Then, given any $C > 0$, there exists a linear state feedback $u = -Kx$ where K only depends on (A, b) and T, μ, M so that, for every M-Lipschitzian (T, μ)-PE signal, the rate of exponential decay of the time-varying system $\dot{x} = (A - \alpha(t)bK)x$ is greater than C.

  In [20] we consider a family of linear control systems $\dot{x} = Ax + \alpha Bu$ where α belongs to a given class of persistently exciting signals. We seek maximal α-uniform stabilisation and destabilisation by means of linear feedbacks $u = Kx$. We extend previous results obtained for bidimensional single-input linear control systems to the general case as follows: if the pair (A, B) verifies a certain Lie bracket generating condition, then the maximal rate of convergence of (A, B) is equal to the maximal rate of divergence of $(-A, -B)$. We also provide more precise results in the general single-input case, where the above result is obtained under the sole assumption of controllability of the pair (A, B).

  The paper [24] considers the stabilization to the origin of a persistently excited linear system by means of a linear state feedback, where we suppose that the feedback law is not applied instantaneously, but after a certain positive delay (not necessarily constant). The main result is that, under certain spectral hypotheses on the linear system, stabilization by means of a linear delayed feedback is indeed possible, generalizing a previous result already known for non-delayed feedback laws.

  Several problems and results related with persistent excitation and stabilization are discussed in the survey [11]. These problems and results deal with both finite- and infinite-dimensional systems.
- In [7] we consider several time-discretization algorithms for singularly perturbed switched systems. The algorithms correspond to different sampling times and the discretization procedure respects the splitting of each mode in fast and slow dynamics. We study whether such algorithms preserve the asymptotic or quadratic stability of the original continuous-time singularly perturbed switched system.
- In [10] we consider affine switched systems as perturbations of linear ones, the equilibria playing the role of perturbation parameters. We study the stability properties of an affine switched system under arbitrary switching, assuming that the corresponding linear system is uniformly exponentially stable. It turns out that the affine system admits a minimal invariant set Ω, whose properties we investigate. In the two-dimensional bi-switched case when both subsystems have non-real eigenvalues we are able to characterize Ω completely and to prove that all trajectories of the system converge to Ω. We also explore the behavior of minimal-time trajectories in Ω by constructing optimal syntheses.
- In [21] we give a collection of converse Lyapunov–Krasovskii theorems for uncertain retarded differential equations. We show that the existence of a weakly degenerate Lyapunov–Krasovskii functional is a necessary and sufficient condition for the global exponential stability of the linear retarded functional differential equations. This is carried out using the switched system transformation approach.

I4S Project-Team

5. New Results

5.1. identification of linear systems

5.1.1. Evaluation of confidence intervals and computation of sensitivities for subspace methods

Participants: Michael Doehler, Laurent Mevel.

Stochastic Subspace Identification methods have been extensively used for the modal analysis of mechanical, civil or aeronautical structures for the last ten years. So-called stabilization diagrams are used, where modal parameters are estimated at successive model orders, leading to a graphical procedure where the physical modes of the system are extracted and separated from spurious modes. Recently an uncertainty computation scheme has been derived allowing the computation of uncertainty bounds for modal parameters at some given model order. In this paper, two problems are addressed. Firstly, a fast computation scheme is proposed reducing the computational burden of the uncertainty computation scheme by an order of magnitude in the model order compared to a direct implementation. Secondly, a new algorithm is proposed to derive the uncertainty bounds for the estimated modes at all model orders in the stabilization diagram. It is shown that this new algorithm is both computationally and memory efficient, reducing the computational burden by two orders of magnitude in the model order[14].

5.1.2. Subspace methods in frequency domain

Participants: Philippe Mellinger, Michael Doehler, Laurent Mevel.

In this paper a combined subspace algorithm and a way to quantify uncertainties of its resulting identified modal parameter has been presented. Even if the algorithm is data-driven, it was proven that uncertainties can still be quantified by using the square subspace matrix without any modification neither on the identified modal parameters or on the stabilization diagrams. A comparison between uncertainty quantification based on this data-driven combined subspace algorithm and the well-known covariance-driven stochastic subspace algorithm shows good results on this new method. Both values and confidence intervals are similar. However combined algorithm gives better results considering spurious modes. [27].

5.1.3. Subspace Identification for Linear Periodically Time-varying Systems

Participants: Laurent Mevel, Ahmed Jhinaoui.

Many systems such as turbo-generators, wind turbines and helicopters show intrinsic time-periodic behaviors. Usually, these structures are considered to be faithfully modeled as Linear Time-Invariant (LTI). In some cases where the rotor is anisotropic, this modeling does not hold and the equations of motion lead necessarily to a Linear Periodically Time-Varying (referred to as LPTV in the control and digital signal field or LTP in the mechanical and nonlinear dynamics world) model. Classical modal analysis methodologies based on the classical time-invariant eigenstructure (frequencies and damping ratios) of the system no more apply. This is the case in particular for subspace methods. For such time-periodic systems, the modal analysis can be described by characteristic exponents called Floquet multipliers. The aim of this paper is to suggest a new subspace-based algorithm that is able to extract these multipliers and the corresponding frequencies and damping ratios. The algorithm is then tested on a numerical model of a hinged-bladed helicopter on the ground. [22], [23], [18].

5.2. damage detection for mechanical structures

5.2.1. Damage detection and localisation

Participants: Michael Doehler, Luciano Gallegos, Laurent Mevel.

Mechanical systems under vibration excitation are prime candidate for being modeled by linear time invariant systems. Damage detection in such systems relates to the monitoring of the changes in the eigenstructure of the corresponding linear system, and thus reflects changes in modal parameters (frequencies, damping, mode shapes) and finally in the finite element model of the structure. Damage localization using both finite element information and modal parameters estimated from ambient vibration data collected from sensors is possible by the Stochastic Dynamic Damage Location Vector (SDDLV) approach. Damage is related to some residual derived from the kernel of the difference between transfer matrices in both reference and damage states and a model of the reference state. Deciding that this residual is zero is up to now done using an empirically defined threshold. In this paper, we show how the uncertainty in the estimates of the state space system can be used to derive uncertainty bounds on the damage localization residuals to decide about the damage location with a hypothesis test.[13], [21], [26].

5.2.2. Robust subspace damage detection

Participants: Michael Doehler, Laurent Mevel.

The detection of changes in the eigenstructure of a linear time invariant system by means of a subspace-based residual function has been proposed previously. While enjoying some success in its applicability in particular in the context of vibration monitoring, the robustness of this framework against changes in the noise properties has not been properly addressed yet. In this paper, a new robust residual is proposed and the robustness of its statistics against changes in the noise covariances is shown. The complete theory for hypothesis testing for fault detection is derived and a numerical illustration is provided[16].

5.2.2.1. Feasibility of reflectometry techniques for non destructive evaluation of external post-tensioned cables

Participant: Qinghua Zhang.

Nowadays a considerable number of bridges is reaching an age when renovating operations become necessary. For some bridges, external post-tension is realized with cables protected in ducts, with the residual internal space imperfectly filled with a fluid cement grout. Detecting the problems of injection in the ducts is visually impossible from the outside. Through a collaboration with the SISYPHE project-team, the feasibility of reflectometry techniques for cable health monitoring is investigated via numerical simulations and laboratory experiments. The main idea consists in adding electrically conductive tapes along a duct so that the duct and the added tapes can be treated as an electrical transmission line. It is then possible to apply advanced reflectometry methods developed by the SISYPHE project-team, initially for true electric cables.

Maxplus Project-Team

6. New Results

6.1. Théorie spectrale max-plus et géométrie métrique/Max-plus spectral theory and metric geometry

6.1.1. Introduction

Participants: Marianne Akian, Stéphane Gaubert, Cormac Walsh.

Étant donné un noyau $a : S \times S \to \mathbb{R} \cup \{-\infty\}$, on peut lui associer le problème spectral max-plus

$$\sup_{y \in S} a(x,y) + u(y) = \lambda + u(x), \quad \forall x \in S, \tag{15}$$

dans lequel on cherche le vecteur propre $u : S \to \mathbb{R} \cup \{-\infty\}$ et la valeur propre correspondante $\lambda \in \mathbb{R} \cup \{-\infty\}$. Comme nous l'avons rappelé dans les §3.2 et 3.3 , le problème spectral (9) intervient en contrôle ergodique: l'ensemble S est l'espace des états, et l'application $a(x,y)$ fournit le gain associé à la transition $x \to y$. Le cas où S est fini est classique, l'on a alors un résultat précis de représentation de l'espace propre, à l'aide d'un certain graphe, dit graphe critique. Des résultats existent également lorsque S est compact et que le noyau vérifie certaines propriétés de régularité.

Dans [61], nous avons considéré le cas où S est non compact. Lorsque $\lambda = 0$, l'espace propre est analogue à l'espace des fonctions harmoniques défini en théorie (classique ou probabiliste) du potentiel. En introduisant l'analogue max-plus de la frontière de Martin, nous avons obtenu un analogue de la formule de représentation de Poisson des fonctions harmoniques : toute solution u de (9) peut être représentée sous la forme :

$$u = \sup_{w \in \mathcal{M}_m} w + \mu_u(w) \ , \tag{16}$$

où $\mathcal{M}_m \subset (\mathbb{R} \cup \{-\infty\})^S$ est l'analogue max-plus de la frontière de Martin minimale (l'ensemble des fonctions harmoniques extrémales normalisées), et où μ_u joue le rôle de la mesure spectrale. Nous avons montré aussi que les éléments de l'espace de Martin minimal peuvent être caractérisés comme les limites de "quasi-géodésiques". La frontière de Martin max-plus généralise dans une certaine mesure la frontière d'un espace métrique construite à partir des horo-fonctions (fonctions de Busemann généralisées), ou horo-frontière. Ces résultats inspirent les travaux des sections suivantes, qui portent sur des cas remarquables d'espaces métriques (§6.1.3) ou sur des applications en théorie des jeux (§6.1.2).

English version

Let the kernel $a : S \times S \to \mathbb{R} \cup \{-\infty\}$ be given. One may associate the max-plus spectral equation (9), where the eigenvector $u : S \to \mathbb{R} \cup \{-\infty\}$ and the eigenvalue $\lambda \in \mathbb{R} \cup \{-\infty\}$ are unknown. As we recalled in §3.2 and refmonotone, this spectral problem arises in ergodic optimal control: the set S is the *state space*, and the map $a(x,y)$ is the *transition reward*. The case when S is finite is classical, a precise spectral theorem is known, with a characterisation of the eigenspace in terms of a critical graph. Some results have been shown when S is compact, assuming that the kernel a satisfies some regularity properties.

In [61], we considered the case where S is non-compact. When $\lambda = 0$, the eigenspace is analoguous to the set of harmonic functions defined in classical or probabilistic potential theory. By introducing a max-plus analogue of the classical Martin boundary, we obtained an analogue of the Poisson representation of harmonic functions, showing that any solution u of (9) may be represented as in (10) where $\mathcal{M}_m \subset (\mathbb{R} \cup \{-\infty\})^S$ is a max-plus analogue of the minimal Martin boundary (the set of normalised extremal harmonic functions), and μ_u plays the role of the spectral measure. We also showed that the elements of the minimal Martin boundary can be characterised as limits of certain "almost-geodesics". The max-plus Martin boundary generalises to some extent the boundary of metric spaces defined in terms of horofunctions (generalised Busemann functions), or horoboundary. These results have inspired the work of the next sections, which deal either with interesting examples of metric spaces (§6.1.3) or with applications to zero-sum games (§6.1.2).

6.1.2. Asymptotiques d'itérées d'applications contractantes au sens large et jeux à somme nulle en horizon long/Asymptotics of iterates of nonexpansive mappings and zero-sum games

Participants: Jérôme Bolte, Stéphane Gaubert, Guillaume Vigeral.

On s'intéresse ici à l'existence du paiement moyen pour les jeux répétés, et plus généralement, à l'existence du vecteur de "taux de fuite" $\lim_k f^k(x)/k$ où f est une application de $\mathbb{R}^n$ dans lui même, nonexpansive pour une norme quelconque. Dans le cas particulier des jeux, f est un opérateur de Shapley, qui est nonexpansif pour la norme sup. On montre dans [45] que la limite existe si l'application f est définissable dans une structure o-minimale. Ceci généralise des résultats de Bewley, Kohlberg, et Neyman, qui montraient que la limite existe si f est semi-algébrique. L'extension au cas o-minimal permet notamment de traiter des opérateurs de type "log-exp" apparaissant en contrôle sensible au risque. Ce travail traite aussi de la question de savoir si un jeu dont les fonctions de paiement et de transition sont définissables dans une structure o-minimale admet un opérateur de Shapley f définissable. Un contre exemple montre que f n'est pas forcément définissable dans la même structure, mais l'on montre qu'il en est ainsi dès que les probabilités de transition ont une structure séparable.

English version

We study the question of the existence of the mean payoff for repeated games, and more generally, the existence of a vector of "escape rates", $\lim_k f^k(x)/k$, where f is a self-map of $\mathbb{R}^n$, non-expansive in some norm. In the special case of zero-sum games, f is a Shapley operator, and it is sup-norm nonexpansive. We showed in [45] that this limit does exist as soon as the map f is definable in an o-minimal structure. This generalizes results of Bewley, Kohlberg, and Neyman, who showed that this limit exists if f is semi-algebraic. The extension to the case of o-minimal structures allows one in particular to deal with log-exp type operators arising in risk sensitive control. This work also adresses the question of knowing whether a game with definable payment and transition functions has a Shapley operator that is definable in the same structure. We gave a counter example showing that this may not be the case, but showed that the Shapley operator is definable as soon as the transition probabilities have a separable structure.

6.1.3. Isométries de la géométrie de Hilbert/Isometries of the Hilbert geometry

Participants: Cormac Walsh, Bas Lemmens [Kent University, UK].

L'un des intérêts de l'horo-frontière est de renseigner sur le groupe des isométries d'un espace métrique. En effet, ce groupe agit naturellement sur l'horo-frontière, et cette action peut parfois être mieux comprise que l'action du groupe sur l'espace d'origine.

Nous avons utilisé ces idées pour étudier le groupe des isométries pour la métrique de Hilbert. De La Harpe [179] a donné plusieurs conjectures relatives à ce groupe. Nous avons montré dans [51], en utilisant l'horo-frontière, que le groupe des isométries est exactement le groupe des transformations linéaires projectives à moins que le domaine ne soit une coupe d'un cône symmétrique non-Lorentzien. Dans ce dernier cas, le groupe linéaire projectif est d'index 2 dans le groupe des isométries. Le cas particulier où le domaine est un polytope a été traité précédemment dans [136].

Dans [51] nous déterminons aussi le groupe des isométries pour une métrique fortement reliée à la métrique de Hilbert, à savoir la métrique de Thompson sur un cone.

English version

One use for the horofunction boundary is to study the group of isometries of a metric space. This is because this group has a well defined action on the horoboundary and it is likely that in many cases this action will be easier to understand than the action on the space itself.

We have been applying these ideas to investigate the isometries of the Hilbert geometry. De La Harpe [179] has previously made several conjectures about the isometry group of this space. We have shown [51] using the horofunction boundary that the isometry group is exactly the group of projective linear transformations unless the domain on which the geometry is defined is a cross section of a non-Lorentzian symmetric cone, in which case the projective linear group is of index two in the isometry group.

The special case when the domain is a polytope was previously considered in [136].

In the paper [51], we also determine the isometry group of closely related metric, the Thompson geometry on a cone.

6.1.4. Consensus non-commutatif et contraction d'opérateurs de Kraus/Noncommutative consensus and contraction of Kraus maps

Participants: Stéphane Gaubert, Zheng Qu.

Dans le travail [47], on s'est intéressé à la vitesse de convergence vers l'équilibre d'une itération de la forme $x^{k+1} = T(x^k)$, $x^k \in X$, où T est une application linéaire préservant un cône dans un espace de Banach X, telle que $T(e) = e$, pour un certain vecteur e dans l'interieur du cône. On s'intéresse aussi à l'itération dans l'espace dual, $y^{k+1} = T^*(y^k)$, $y^k \in X^*$, lorsque $\langle y^0, e\rangle = 1$.

Le cas classique est celui où $T(x) = Px$ est un opérateur de Markov. L'itération primale traduit alors la convergence vers le "consensus", et l'itération duale traduit la convergence de la distribution de probabilité en temps k vers l'état stationnaire. Dans ce cas, le taux de contraction (en un coup) $\kappa(P)$ d'une itération primale, pour la semi-norme de Hilbert $\|z\|_H := \max_i z_i - \min_j z_j$, ainsi que le taux de contraction d'une itération duale, pour la métrique en variation totale, coïncident et sont caractérisés par une formule dûe à Doeblin et Dobrushin (coefficient d'ergodicité),

$$\kappa(P) := 1 - \min_{i,j} \sum_{s=1}^{n} \min\left(P_{is}, P_{js}\right).$$

On a donné ici une généralisation de cette formule au cas d'opérateurs abstraits, qui s'applique en particulier aux opérateurs de Kraus qui interviennent en information quantique. Ces derniers opérent sur l'espace des matrices symmétriques, et sont de la forme

$$T(x) = \sum_k a_k x a_k^* \qquad \text{avec} \qquad \sum_k a_k a_k^* = I \ .$$

Dans [34], nous avons étendu ces résultats aux flots non-linéaires sur les cones.

English version

In a recent work [27], we studied the speed of convergence to equilibrium of an iteration of the form $x^{k+1} = T(x^k)$, $x^k \in X$, where T is a linear map preserving a cone in a Banach space X, such that $T(e) = e$, for some vector e in the interior of the cone. We also considered the iteration in the dual space X^*, $y^{k+1} = T^*(y^k)$, $y^k \in X^*$, where $\langle y^0, e\rangle = 1$.

The classical application arises when $T(x) = Px$ is a Markov operator. Then, the primal iteration represents the dynamics of consensus, whereas the dual iteration represents the evolution of the probability distribution as a function of time. Then, the (one-shot) contraction rate $\kappa(P)$ of the primal iteration, with respect to Hilbert's seminorm $\|z\|_H := \max_i z_i - \min_j z_j$, and the contraction rate of the dual iteration, with respect to the total variation metric, coincide, and are characterized by a formula of Doeblin and Dobrushin (ergodicity coefficient),

$$\kappa(P) := 1 - \min_{i,j} \sum_{s=1}^{n} \min(P_{is}, P_{js}).$$

We gave here a generalization of this formula to an abstract operators on a cone. This covers in particular the Kraus maps arising in quantum information theory. The latter maps act on the space of symmetric matrices. They can be written as

$$T(x) = \sum_k a_k x a_k^* \qquad \text{with} \qquad \sum_k a_k a_k^* = I \ .$$

In [34], we generalized these results to non-linear flows over cones.

6.2. Algèbre linéaire max-plus et convexité abstraite/Max-plus linear algebra and abstract convex analysis

6.2.1. Convexité max-plus ou tropicale/Max-plus or tropical convexity

Participants: Xavier Allamigeon, Stéphane Gaubert, Eric Goubault [CEA], Ricardo Katz [Conicet, Argentine].

On étudie les analogues max-plus ou tropicaux des ensembles convexes. Ceux-ci sont utiles en particulier pour représenter de manière effective les ensembles d'états accessibles de systèmes à événements discrets [9], ils sont aussi apparus récemment en géométrie tropicale, dans toute une série de travaux à la suite de Sturmfels et Develin [96]. Les polyèdres max-plus peuvent aussi être vus comme des limites de déformations de polyèdres classiques, sur lesquels ils donnent un éclairage de nature combinatoire. Toutes ces motivations ont inspiré la recherche d'analogues des résultats fondamentaux d'analyse convexe classique: séparation, projection, points extrémaux, à la suite en particulier de [8].

Dans un travail de X. Allamigeon, S. Gaubert, et E. Goubault [64], [16], on a mis en évidence un critère combinatoire pour la caractérisation des sommets des polyèdres tropicalement convexes. Celui-ci s'exprime à l'aide d'hypergraphes orientés, et de leurs composantes fortement connexes. Ce critère possède la propriété d'être vérifiable en un temps presque linéaire en la taille de l'hypergraphe.

On en déduit un analogue tropical de la méthode de la double description [16] (méthode très utilisée sur les polyèdres classiques, et dûe à Motzkin *et al.* [148]). Cet algorithme permet de calculer les sommets d'un polyèdre défini de façon externe (intersection de demi-espaces ou d'hyperplans tropicaux). Grâce au critère combinatoire précédent, l'algorithme améliore de plusieurs ordres de grandeur les techniques connues jusqu'alors. Ceci est confirmé par de nombreuses expérimentations. Ce travail est motivé par des applications à l'analyse statique [63] et aux systèmes à événements discrets [99], dans lesquelles la manipulation de tels polyèdres est le goulot d'étranglement.

Il est connu qu'un polyèdre tropical peut être représenté comme l'enveloppe convexe d'un ensemble minimal de points et rayons, donnés par ses sommets et ses rayons extrêmes [111]. Dans un travail réalisé par X. Allamigeon et R. Katz [17], et effectué en partie lors de visites de R. Katz à Inria, on étudie la question duale de la caractérisation des représentations minimales par demi-espaces. On montre qu'un polyèdre tropical possède *essentiellement* une unique représentation minimale par demi-espaces, lorsque leurs apex appartiennent au polyèdre. On montre que les apex de ces demi-espaces non-redondants correspondent à certains sommets du complexe tropical introduit par Develin et Sturmfels [96]. On introduit également un critère combinatoire pour l'élimination de demi-espaces redondants à l'aide d'hypergraphes orientés.

Dans un travail en cours de X. Allamigeon, P. Benchimol, S. Gaubert et R. Katz, nous étudions la tropicalisation des représentations par demi-espaces des polyèdres convexes sur le corps des séries de Puiseux. Nous démontrons ainsi une conjecture de Develin et Yu [97]. Celle-ci assure qu'étant donné un polytope tropical pur, il existe un polytope *relevé* sur les séries de Puiseux, dont les demi-espaces associés aux faces se "tropicalisent" en une représentation par demi-espaces du polytope tropical initial.

Des applications de ces travaux à l'algorithmique, concernant en particulier les jeux répétés, sont discutées dans la Section 6.4.2 . Une application aux systèmes temps réel est discutée dans la Section 6.5.4 .

English version

We study the max-plus or tropical analogues of convex sets. These have been used in particular to represent effectively the accessible sets of certain discrete event systems [9]. They also appeared in tropical geometry, following the work of Sturmfels and Develin [96]. Max-plus polyhedra can be thought of as limits of deformations of classical polyhedra, on which they give a combinatorial insight. These motivations have inspired the investigation of analogues of basic results of classical convex analysis: separation, projection, representation by extreme points, following [8].

In a work of X. Allamigeon, S. Gaubert, and E. Goubault [16], we introduce a combinatorial criterion for the characterization of the vertices of tropically convex polyhedra. It is expressed in terms of directed hypergraphs and their strongly connected components. This criterion can be verified in almost linear time in the size of the hypergraph.

This allows to develop a tropical analogue of the double description method [16] (this method is widely used for classical convex polyhedra, and is due to Motzkin *et al.* [148]). This algorithm is able to determine all the vertices of a polyhedron defined externally (intersection of tropical half-spaces of hyperplanes). Thanks to the combinatorial criterion mentioned above, the algorithm improves the existing methods by several orders of magnitude. This is confirmed by several experiments. This is motivated by applications to static analysis [63] and discrete event systems [99], in which computing such polyhedra turns out to be the bottleneck.

It is well-known that a tropical polyhedron can be represented as the convex hull of a minimal set of points and rays, provided by its vertices and extreme rays [111]. In a work of X. Allamigeon and R. Katz [17], partly done during visits of R. Katz at Inria, the dual problem of characterizing the minimal representations by half-spaces is studied. We show that a tropical polyhedron admits *essentially* a unique minimal external representation by half-spaces, provided that their apices belong to the polyhedron. We prove that the apices of these half-spaces correspond to certain vertices of the tropical complex introduced by Develin and Sturmfels [96]. We also establish a combinatorial criterion allowing to eliminate redundant half-spaces using directed hypergraphs.

In an ongoing work of X. Allamigeon, P. Benchimol, S. Gaubert and R. Katz, we study the tropicalization of the representation by half-spaces of convex polyhedra over the field of Puiseux series. In particular, we prove a conjecture of Develin and Yu [97]. It states that, given a pure tropical polytope, there exists a lifting polytope over Puiseux series, such that the facet-defining half-spaces are "tropicalized" into a representation by half-spaces of the initial polytope.

Some algorithmic applications of this work concerning in particular mean payoff games, will be discussed in Section 6.4.2 . Applications to real time systems will be discussed in Section 6.5.4 .

6.2.2. Systèmes linéaires max-plus/Max-plus linear systems

Participants: Marianne Akian, Stéphane Gaubert, Alexander Guterman [Moscow State University].

Dans [37], on montre des formules de Cramer pour des systèmes linéaires sur diverses extensions du semi-anneau max-plus. Les éléments de ces extensions sont des nombres tropicaux enrichis d'une information de multiplicité, de signe ou d'angle par exemple. On obtient ainsi des résultats d'existence et d'unicité qui généralisent plusieurs résultats de [121], [153], [107], [161], [127]. De plus, pour certaines extensions du semi-anneau max-plus, les preuves fournissent des algorithmes de type Jacobi ou Gauss-Seidel pour résoudre les systèmes linéaires.

English version

In [37], we prove general Cramer type theorems for linear systems over various extensions of the tropical semiring, in which tropical numbers are enriched with an information of multiplicity, sign, or argument. We obtain existence or uniqueness results, which extend or refine earlier results in [121], [153], [107], [161], [127]. Moreover, some of our proofs lead to Jacobi and Gauss-Seidel type algorithms to solve linear systems in suitably extended tropical semirings.

6.3. Algèbre max-plus, déformations et asymptotiques /Max-plus algebra, deformations and asymptotic analysis

6.3.1. Introduction

Comme indiqué dans le §3.7 , l'algèbre max-plus est la limite d'une déformation de l'algèbre classique, ou plutôt du semi-corps des réels positifs. Elle peut aussi fournir des estimations de ces déformations, puisque

$$\max(a,b) \leq \epsilon \log\left(e^{a/\epsilon} + e^{b/\epsilon}\right) \leq \epsilon \log(2) + \max(a,b) \ . \tag{17}$$

L'utilisation de ces propriétés a déjà conduit dans le passé aux travaux sur les perturbations de valeurs propres [55], [54], [53], ou sur les grandes déviations [1], [59]. Dans les travaux qui suivent, nous exploitons ces propriétés dans des contextes reliés ou similaires à ceux de nos travaux précédents.

English version

As detailled in §3.7 , max-plus algebra is the limit of a deformation of classical algebra, or more precisely of the semi-field of usual real positive numbers. It can also give estimations for these deformations using for instance (11). By using these properties, we already obtained some works on singular perturbations of matrix eigenvalues [55], [54], [53], or on large deviations [1], [59]. In the works described below, we are exploiting again these properties in contexts that are related or similar to those of our earlier works.

6.3.2. Aspects tropicaux des algorithmes de scaling matriciel/Tropical aspects of matrix scaling problems

Participants: Marianne Akian, Stéphane Gaubert, Meisam Sharify Najafabadi [Univ. Manchester].

Une partie du travail de thèse de M. Sharify [167] portait sur les méthodes de mise à l'échelle pour améliorer la précision du calcul de valeurs propres. En appliquant les techniques de [53], [54], on montrait notamment que l'ordre de grandeur des valeurs propres d'un faisceau matriciel est donné (sous des conditions de non-dégénérescence) par les valeurs propres tropicales, qui peuvent être calculées de manière robuste, et fournissent ainsi une mise à l'échelle pour calculer les valeurs propres classiques.

Nous avons poursuivi ce travail dans [41]. On calcule cette fois l'ordre de grandeur des valeurs propres d'un polynôme matriciel au moyen des racines tropicales du polynôme obtenu en appliquant une norme donnée aux coefficients. Les racines dépendent de la norme choisie, et la norme de Frobenius est optimale en un certain sens. On obtient des bornes générales pour les ratios entre modules des valeurs propres et racines tropicales qui généralisent les bornes obtenues par Polya et Ostrowski dans le cas de polynômes scalaires. On raffine aussi ces bornes, en particulier lorsque les racines tropicales sont bien séparées les unes des autres.

English version

A part of the PhD work of M. Sharify [167] dealt with scaling methods to improve the accuracy of eigenvalue numerical computions. Applying the techniques of [53], [54], we showed in particular that the order of magnitude of the eigenvalues of a matrix pencil can be determined (under nondegeracy conditions) by computing tropical eigenvalues. The latter can always be computed accurately and provide a scaling which can be combined with standard numerical methods for matrix pencils.

We have pursued this work in [41]. Now, we compute the order of magnitude of the eigenvalues of a matrix polynomial by using the tropical roots of a polynomial obtained by applying a norm to the coefficients of the original matrix polynomial. The tropical roots depend on the chosen norm, and the Frobenius turns out to be optimal in a certain sense. We obtain indeed general bounds on the ratios between the modulus of the eigenvalues of the matrix polynomial and the tropical roots which generalize the bounds of Polya and Ostrowski available for scalar polynomials. We also improve these bounds, in particular when the tropical roots are well separated.

6.3.3. *Méthodes tropicales de localisation de valeurs propres de matrices/Tropical methods for the localisation of matrix eigenvalues*

Participants: Marianne Akian, Stéphane Gaubert, Andrea Marchesini.

Le travail de stage de M2 d'Andrea Marchesini a conduit à la publication [14] dans laquelle on montre des inégalités de type majorisation entre les valeurs propres d'une matrice et les valeurs propres tropicales de la matrice de ses modules. En particulier, la majoration est une généralisation de l'inégalité de Friedland [106] concernant le rayon spectral.

La thèse d'Andrea Marchesini s'inscrit dans le prolongement de son stage de M2 dans l'équipe et certains des travaux de la thèse de Meisam Sharify [167]. Le but est d'obtenir des inégalités de type majorisation permettant d'estimer a priori les valeurs propres de matrices ou de faisceaux de matrices, en faisant éventuellement intervenir des hypothèses de bon conditionnements. En particulier on recherche la localisation de ces valeurs propres en fonction de valeurs propres de matrices agrégées ou simplifiées. On cherchera aussi à obtenir le même type de localisation ou d'estimation dans le cas des vecteurs propres associés, par exemple en utilisant les techniques de compléments de Schur de [54] ou les idées de Murota [149].

L'idée est ensuite d'utiliser ces résultats de localisation pour améliorer la précision des algorithmes de calcul numérique de valeurs propres de matrices, en particulier en construisant des changements d'échelle exploitant les calculs tropicaux, à effectuer préalablement à l'appel d'algorithmes classiques comme QZ. Les travaux de Stéphane Gaubert et Meisam Sharify [115] ont montré l'intérêt de cette approche, notamment pour les problèmes de faisceaux quadratiques de valeurs propres issus de systèmes mécaniques pour lesquels on dispose de nombreux exemples pathologiques pour les algorithmes existants. Dans un travail en collaboration avec Françoise Tisseur et James Hook de l'Université de Manchester, on montre l'intérêt des changements d'échelle en termes de le conditionnement des valeurs propres.

English version

The M2 internship of Andrea Marchesini led to the publication [14], in which we show majorization type inequalities between the eigenvalues of a matrix and the tropical eigenvalues of the matrix obtained by applying the modulus entrywise. In particular, the bound is a generalization of the inequality of Friedland [106] concerning the spectral radius.

The PhD thesis follows his M2 internship and some of the works of Meisam Sharify's PhD thesis [167]. The aim is to obtain majorization type inequalities allowing one to estimate the eigenvalues of matrices or matrix polynomials, using possibly assumptions on condition numbers. In particular, one may look for estimates of these eigenvalues using the eigenvalues of aggregated or simplified matrices. One may also try to find the same type of estimates for the associated eigenvectors, for instance by using techniques of Schur complements from [54] or ideas of Murota [149].

One would like to use these estimation results to improve the accuracy of eigenvalue numerical computions, in particular by constructing scaling methods using tropical techniques, which may be used before calling usual algorithms as QZ. The works of Stéphane Gaubert and Meisam Sharify [115] showed the interest of this approach, in particular for quadratic matrix polynomials issued from mechanical systems for which there exists several pathological examples for existing algorithms. In a work with Françoise Tisseur and James Hook from Manchester University, we show the interest of these scaling methods on the eigenvalue conditioning.

6.3.4. *Mesures et applications maxitives/Maxitive measures and maps*

Participants: Marianne Akian, Stéphane Gaubert, Paul Poncet.

La thèse de Paul Poncet [154] concernait essentiellement ce que l'on appelle l'analyse idempotente, c'est-à dire l'étude des espaces fonctionnels ou linéaires de dimension infinie sur l'algèbre tropicale, ou tout autre semi-anneau idempotent. Paul Poncet a développé pour cela un point de vue treillis continus comme dans [1], ou plus généralement domaines. Depuis la soutenance, plusieurs articles issus du manuscrit de thèse sont en cours de publication ou de soumission, et d'autres travaux pousuivant ceux de la thèse sont en cours avec les membres de l'équipe.

La première partie de la thèse traitait des mesures maxitives, en particulier de l'existence d'une densité cardinale ou d'une densité d'une mesure par rapport à une autre (théorème de Radon-Nikodym), et de la régularité d'une mesure maxitive. Ces travaux sont publiés ou en cours de publication dans [49] et [23] respectivement.

La deuxième partie concernait les convexes dans les semi-treillis ou l'algèbre max-plus, pour lesquels Paul Poncet a pu établir des théorèmes de type Krein-Milman, réciproque de Milman, et représentation de Choquet. [48] traite du cas des semi-treillis.

On sait que les résultats sur les convexes tropicaux de dimension infinie de [154] permettent de retrouver partiellement les résultats sur la frontière de Martin max-plus décrits dans la section 6.1.1 . Dans un travail commun nous essayons d'obtenir d'autres applications et extensions du théorème de représentation de Choquet tropical. En particulier on considère le cas d'ensembles ordonnés qui ne sont pas forcément des treillis tels que le cône des matrices symmetriques positives muni de l'ordre de Loewner.

English version

The PhD thesis work of Paul Poncet [154] concerned essentially what is called idempotent analysis, that is the study of infinite dimensional functional or linear spaces over tropical algebra, or any other idempotent semiring. For this aim, Paul Poncet developped the point of view of continuous lattices, as in [1], or more generally of domains. Since the defense of his thesis, several papers derived from the thesis manuscript have been submitted and some are published or up to be published. Some other works pursuing the thesis work are done with team members.

The first part of the Paul Poncet's thesis concerned maxitive measures, in particular the existence of a cardinal density of a measure, or that of a density of a measure with respect to another (Radon-Nikodym theorem), and the regularity of a maxitive measure. These works are now published or accepted for publication in [49] and [23] respectively.

A second part concerned convex sets in lattices or max-plus algebra, for which Paul Poncet showed results such as a Krein-Milman type theorem, a Milman converse type theorem, and a Choquet representation type theorem. [48] concerns the case of semilattices.

We know that the results on infinite dimensional tropical convex sets of [154] allow one to recover at least partially the results on max-plus Martin boundaries described in Section 6.1.1 . In a joint work, we try to obtain other applications and extensions of the max-plus Choquet representation theorem. In particular, we consider the case of ordered sets that are not necessarily semilattices, such as the cone of nonnegative symmetric matrices endowed with the Loewner order.

6.4. Algorithmes/Algorithms

6.4.1. Itération sur les politiques pour le contrôle stochastique et les jeux répétés à somme nulle/Policy iterations for stochastic control and repeated zero sum games

Participants: Marianne Akian, Jean Cochet-Terrasson [CGA], Sylvie Detournay, Stéphane Gaubert.

L'algorithme d'itération sur les politiques est bien connu pour résoudre efficacement les équations de la programmation dynamique associées à des problèmes de contrôle stochastique avec critère à horizon infini (Howard) ou ergodique (Howard, et Denardo et Fox). Récemment, il a été généralisé au cas de problèmes de jeux à deux joueurs et somme nulle dégénérés (avec paiements ergodiques et de type "multi-chaîne"), au moyen de techniques d'algèbre max-plus et de théorie du potentiel non linéaire [84]. Chaque itération de base

de cet algorithme utilise la résolution d'un système d'équations linéaires dont l'opérateur est monotone, mais dont la taille peut être grande, soit parce qu'il provient d'une discrétisation fine d'une équation aux dérivées partielles, soit parce qu'il est associé à un problème discret de grande taille comme le graphe du Web.

La thèse de Sylvie Detournay [95] a permis de développer et d'étudier un algorithme associant une méthode d'itération sur les politiques du type de celle introduite par Cochet-Terrasson et Gaubert dans [84] et une méthode multigrille algèbrique, afin de résoudre des problèmes de jeux à somme nulle dégénérés, éventuellement posés directement sous forme discrète. L'ensemble des codes nouveaux associés, écrits en C, est déposé sur le projet "pigames" de la gforge et sera disponible librement.

Sylvie Detournay a en particulier implémenté et raffiné l'algorithme proposé dans [84], en l'associant soit à des méthodes de résolution exacte de systèmes linéaires, soit à des méthodes multigrilles algébriques, en utilisant aussi des méthodes multigrilles multiplicatives pour le calcul de la mesure invariante de chaînes de Markov irréductibles, comme celles introduites par De Sterck. Ceci a permis l'obtention de résultats numériques dans le cas de discrétisations d'équations d'Isaacs associées à des jeux de poursuite déterministes ou aléatoires. Cela a aussi permis de tester de manière systématique l'algorithme sur des instances aléatoires de jeux de type Richman. Certains de ces résultats, ainsi que la présentation de l'algorithme (de manière plus concrète que dans [84], et avec les détails d'implémentation) sont présentés dans [24]. Des details supplémentaires ainsi que la preuve de convergence de l'algorithme peuvent être trouvés dans [56].

Des résultats récents de Ye ainsi que Hansen, Miltersen et Zwick montrent que l'algorithme d'itération sur les politiques, restreint à la classe des jeux à somme nulle (à 1 ou 2 joueurs) actualisés de facteur d'actualisation donné, est fortement polynomial. Dans [40], [29], on montre que ceci est le cas aussi pour l'algorithme d'itération sur les politiques pour les jeux à somme nulle et paiement moyen, restreint à la classe des jeux qui ont temps moyen de retour ou d'arrivée à un état donné borné. La preuve utilise des techniques de théorie de Perron-Frobenius non-linéaire, permettant de ramener le problème à paiement moyen à un problème actualisé (de facteur d'actualisation dépendant de l'état et des actions). La même technique permet aussi de traiter le cas de jeux à somme nulle actualisés dont le facteur d'actualisation peut dépendre de l'état et des actions et prendre éventuellement des valeurs supérieures à 1.

English version

Policy iteration is a powerful and well known algorithm to solve the dynamic programming equation associated to stochatic control (one player game) problems with infinite horizon criterion (Howard) or ergodic criterion (Howard and Denardo and Fox). It has recently been extended to degenerate two players problems (with ergodic payoff and in "multichain" cases) using ideas from max-plus algebra and nonlinear potential theory [84]. One basic iteration of the algorithm consists in solving a linear system the operator of which is monotone, but with a size which may be large since it comes from the discretization of a partial differential equation or since it is associated to a large size discrete problem arising from instance from the Web graph.

The PhD thesis of Sylvie Detournay [95] developped and studied an algorithm for degenerate two player games (that may come from a discrete time and finite state space model) combining a policy iteration such as the one introduced in [84] by Cochet-Terrasson et Gaubert, and an algebraic multigrid method (AMG). All new corresponding algorithms, coded in C, belong to the gforge project "pigames" and will be distributed openly.

In particular, Sylvie Detournay has implemented and refined the algorithm proposed in [84], while associating it either to direct linear solvers, or to the AMG methods already used in the nondegenerate case, and using also multiplicative AMG methods for computing invariant measures of Markov chains, such as the one introduced by De Sterck. This allowed her to obtain numerical results in the case of discretisations of Isaacs equations associated to deterministic or stochastic pursuit games. This also allowed her to test systematically the algorithm on random instances of Richman type games.

Some of these results, together with the presentation of the algorithm (in a more practical manner than in [84], with implementation details) are gathered in [24]. Additional details and the convergence proof of the algorithm can be found in [56].

Recent results of Ye and Hansen, Miltersen and Zwick show that policy iteration for one or two player (perfect information) zero-sum stochastic games, restricted to instances with a fixed discount rate, is strongly polynomial. In [40], [29], we show that policy iteration for mean-payoff zero-sum stochastic games is also strongly polynomial when restricted to instances with bounded first mean return time to a given state. The proof is based on methods of nonlinear Perron-Frobenius theory, allowing us to reduce the mean-payoff problem to a discounted problem with state dependent discount rate. Our analysis also shows that policy iteration remains strongly polynomial for discounted problems in which the discount rate can be state dependent (and even negative) at certain states, provided that the spectral radii of the nonnegative matrices associated to all strategies are bounded from above by a fixed constant strictly less than 1.

6.4.2. Algorithmique des polyèdres tropicaux/Algorithmics of tropical polyhedra

Participants: Xavier Allamigeon, Pascal Benchimol, Stéphane Gaubert, Eric Goubault [CEA], Michael Joswig [TU Darmstadt].

X. Allamigeon, S. Gaubert, et E. Goubault, ont développé dans [63], [16] plusieurs algorithmes permettant de manipuler des polyèdres tropicaux. Ceux-ci correspondent aux travaux décrits dans §6.2.1 . Ils permettent notamment de déterminer les sommets et rayons extrêmes d'un polyèdre tropical défini comme intersection de demi-espaces, ou inversement, de calculer une représentation externe à partir d'un ensemble de générateurs. Ces algorithmes sont implémentés la bibliothèque TPLib (voir §5.3).

Dans un travail en cours de X. Allamigeon, P. Benchimol, S. Gaubert et M. Joswig, nous avons défini un analogue tropical de l'algorithme du simplexe qui permet de résoudre les problèmes de *programmation linéaire tropicale*, *i.e.*

$$\begin{aligned} \text{minimiser} \quad & \max_{1\le j\le n} c_j + x_j \\ \text{sous les contraintes} \quad & \max\big(\max_{1\le j\le n}(a^+_{ij}+x_j), b^+_i\big) \ge \max\big(\max_{1\le j\le n}(a^-_{ij}+x_j), b^-_i\big), \quad i=1,\cdots,m \\ & x \in (\mathbb{R}\cup\{-\infty\})^n \end{aligned} \tag{18}$$

où les entrées du programme $a^{\pm}_{ij}$, $b^{\pm}_i$, c_j sont à valeur dans $\mathbb{R}\cup\{-\infty\}$. Ces problèmes sont intimement liés à la résolution de jeux répétés à somme nulle, puisque résoudre un jeux à paiement moyen déterministe est équivalent à déterminer si un problème de programmation linéaire admet un point réalisable [57].

Comme son homologue usuel, le simplexe tropical pivote entre des points de base (tropicaux), jusqu'à atteindre l'optimum du programme linéaire. La différence fondamentale avec l'algorithme du simplexe classique est que le pivotage est réalisé de manière purement combinatoire, en s'appuyant sur des descriptions locales du polyèdre tropical défini par les contraintes à l'aide d'(hyper)graphes orientés. Ceci nous a permis de prouver que *l'étape de pivotage (incluant le calcul des coûts réduits) a la même complexité en temps que dans l'algorithme classique, i.e.* $O(n(m+n))$. Ceci est d'autant plus inattendu que la structure des arêtes tropicales entre deux points de base sont géométriquement plus complexes (elles sont constituées de plusieurs segments de droite, jusqu'à n).

Le simplexe tropical a la propriété d'être fortement corrélé avec l'algorithme du simplexe classique. Grâce au principe de Tarski, le simplexe usuel peut être transposé tel quel sur des programmes linéaires dont les coefficients en entrée sont non plus des réels, mais sur le corps $\mathbb{R}\{\{t\}\}$ des séries de Puiseux généralisées en une certaine indéterminée t, *i.e.* des objets de la forme :

$$c_{\alpha_1} t^{\alpha_1} + c_{\alpha_2} t^{\alpha_2} + \cdots \tag{19}$$

où les α_i sont des réels, les coefficients c_{α_i} sont des réels non-nuls, et où la séquence des $\alpha_1, \alpha_2, \cdots$ est strictement croissante et soit finie, soit non-bornée. L'opposé du plus petit exposant de la série, $-\alpha_1$, est appelé *valuation* de la série. Un programme linéaire tropical est dit *relevé* en un problème linéaire sur $\mathbb{R}\{\{t\}\}$, si la valuation des coefficients en entrée de ce dernier sont égaux aux coefficients du problème tropical. Dans nos travaux, nous avons établi la correspondance suivante entre le simplexe usuel et le simplexe tropical : *pour tout programme linéaire tropical générique, l'algorithme du simplexe tropical trace l'image par la valuation du chemin sur l'algorithme du simplexe usuel sur n'importe quel relèvement du programme tropical dans* $\mathbb{R}\{\{t\}\}$.

Les résultats présentés ci-dessus sont rassemblés dans le preprint [43]. Ils ont fait l'objet de plusieurs présentations en conférence [32], [33].

Ces résultats ouvrent la possibilité de relier la complexité du l'algorithme du simplexe usuel avec celles des jeux déterministes. Pour ces derniers, on sait seulement que leur résolution est dans la classe de complexité $\mathsf{NP} \cap \mathsf{coNP}$, et on ignore s'il existe un algorithme de complexité polynomiale. De façon similaire, on ne sait pas caractériser de façon précise la complexité de l'algorithme du simplexe usuel. Celle-ci dépend fortement de la règle de pivotage utilisée, et il existe des problèmes sur lesquelles de nombreuses règles de pivotage ont une complexité exponentielle. L'existence d'une règle de pivotage qui permettrait au simplexe de terminer en temps polynomial sur n'importe quelle instance est encore aujourd'hui une question ouverte.

Dans un deuxième travail, nous avons relié les deux problèmes ouverts précédents, grâce à l'algorithme du simplexe tropical. Nous avons en effet exhibé une classe de règles de pivotage, dites *combinatoires*, et avons montré qu'elles satisfont la propriété suivante : *s'il existe une règle de pivotage combinatoire qui permet de résoudre tout problème de programmation linéaire usuel en temps polynomial, alors on peut résoudre les jeux à paiement moyen en temps (fortement) polynomial.* Le terme *combinatoire* fait référence au fait que la règle est définie en fonction du signe des mineurs de la matrice des coefficients du problème linéaire.

Ce dernier résultat est décrit dans le preprint [42].

English version

X. Allamigeon, S. Gaubert, and E. Goubault, have developed in [63], [16] algorithms allowing one to manipulate tropical polyhedra. They correspond to the contributions described in §6.2.1 . In particular, they can be used to determine the vertices and extreme rays of a tropical polyhedron defined as the intersection of half-spaces, or inversely, to compute an external description from a set of generators. These algorithms are implemented in the library TPLib (see §5.3).

In an ongoing work of X. Allamigeon, P. Benchimol, S. Gaubert and M. Joswig, we introduced a tropical analogue of the simplex algorithm, allowing one to solve problems of *tropical linear programming*, which are of the form (12), where the coefficients of the program, $a_{ij}^{\pm}$, $b_i^{\pm}$, c_j take their values in the max-plus semiring $\mathbb{R} \cup \{-\infty\}$. These problems are closely related to mean payoff games, as solving a game of this kind is equivalent to determine whether a tropical linear program admits a feasible point [57].

Like the classical simplex algorithm, the tropical simplex algorithm performs pivoting operations between basis points, until it reaches the optimum. The main discrepancy with the classical algorithm is that the pivoting is now a purely combinatorial operation, which is performed by using a local description of the polyhedron by a directed hypergraph. This allowed us to show that *a tropical pivoting step (including computing reduced costs) has the same complexity as in the classical simplex algorithm, i.e.* $O(n(m+n))$. This is all the more surprising as the tropical edge between two given points has a geometrically more complex structure in the tropical case (it is constituted of up to n ordinary line segments).

The tropical simplex algorithm turns out to be closely related to the classical one. Thanks to Tarski's principle, the latter is also valid for linear programs over the field $\mathbb{R}\{\{t\}\}$ of generalized Puiseux series in an indeterminate t. These series are of the form (13), where the α_i are real numbers, the coefficients c_{α_i} are non-zero reals, and the sequence $\alpha_1, \alpha_2, \cdots$ is strictly increasing and either finite or unbounded. The opposite of the smallest exponent of the series, $-\alpha_1$, is called *valuation*. A tropical linear program is said to be *lifted* to a linear program over $\mathbb{R}\{\{t\}\}$ if the valuation of the coefficients of the latter are sent to the coefficients of

the former by the valuation. We showed the following relation between the classical simplex algorithm and its tropical analogue: *for all generic tropical linear program, the tropical simplex algorithm computes the image by the valuation of the path of the classical simplex algorithm, applied to any lift in* $\mathbb{R}\{\{t\}\}$ *of the original program*.

These results are gathered in the preprint [43]. They have been presented in several conferences [32], [33].

They allow one to relate the complexity of the classical simplex algorithm with the complexity of mean payoff games. The latter is unsettled, these games are known to be in the class $\mathsf{NP} \cap \mathsf{coNP}$ but it is not known whether they can be solved in polynomial time. Basic complexity issues regarding the classical simplex algorithm are also unsettled: its execution time depends on the pivoting rule, and many pivoting rules have been shown to have exponential worst case behaviors. The existence of a pivoting rule leading the simplex to terminate in polynomial time is still an open question.

In a second work, we related these two open questions, via the tropical simplex algorithm. We identified a class of pivoting rules, which are said to be *combinatorial*, and show that they have the following property: *if there is a combinatorial pivoting rule allowing one to solve every classical linear programming problem in polynomial time, then, mean payoff games can be solved in (strongly) polynomial time.* By *combinatorial*, we mean that the rule depends only of the coefficients of the system through the signs of minors of the coefficients matrix.

This result is given in the preprint [42].

6.4.3. Problèmes d'accessibilité dans les hypergraphes orientés et leur complexité/Reachability problems in directed hypergraphs and their complexity

Participant: Xavier Allamigeon.

Les hypergraphes orientés sont une généralisation des graphes orientés, dans lesquelles chaque arc relie un ensemble de sommets à un autre. Ils jouent un rôle important dans les travaux récents sur la convexité tropicale (voir §6.2.1), puisqu'ils offrent une représentation naturelle des cônes définis sur le sous-semi-anneau booléen $\mathbb{B} = \{-\infty, 0\}$.

Dans un travail de X. Allamigeon [15], on étudie la complexité de problèmes d'accessibilité sur les hypergraphes orientés. Nous introduisons un algorithme de complexité presque linéaire permettant de déterminer les composantes fortement connexes terminales (qui n'accèdent à aucune autre composante si ce n'est elles-mêmes) d'un hypergraphe.

Nous établissons également une borne inférieure sur-linéaire sur la taille de la réduction transitive de la relation d'accessibilité dans les hypergraphes. Cela indique que la relation d'accessibilité dans les hypergraphes orientés est combinatoirement plus complexe que celle des graphes orientés. Cela suggère aussi que des problèmes comme le calcul des composantes fortement connexes est plus difficile sur les hypergraphes que sur les graphes. Nous mettons d'ailleurs en évidence une réduction en temps linéaire du problème du calcul des ensembles minimaux dans une famille d'ensembles donnée, vers le problème du calcul de toutes les composantes fortement connexes d'un hypergraphe. Le problème du calcul des ensembles minimaux a été largement étudié dans la littérature [155], [175], [174], [156], [157], [158], [101], [69], et aucune algorithme en temps linéaire n'est connu à ce jour.

English version

Directed hypergraphs are a generalization of directed graphs, in which the tail and the head of the arcs are sets of vertices. It appears that they play an important role in the recent works on tropical convexity (see §6.2.1), since they offer a natural representation of cones defined over the boolean sub-semiring $\mathbb{B} = \{-\infty, 0\}$.

In a work of X. Allamigeon [15], we study the complexity of reachability problems on directed hypergraphs. We introduce an almost linear-time algorithm allowing to determine the terminal strongly connected components (a component is said to be *terminal* when no other component is reachable from it).

We also establish a super-linear lower bound over the size of the transitive reduction of the reachability relation in directed hypergraphs. This indicates that the reachability relation is combinatorially more complex in directed hypergraphs than in directed graphs. This also suggests that reachability problems such as computing all strongly connected components are likely to be harder in hypergraphs than in graphs. Besides, we show that the minimal set problem can be reduced in linear time to the problem of computing all strongly connected components in hypergraphs. The former problem consists in finding all minimal sets among a given family of sets. It has been well studied in the literature [155], [175], [174], [156], [157], [158], [101], [69], and no linear time algorithm is known.

6.4.4. *Approximation max-plus de fonctions valeurs et équations de Riccati généralisées/Max-plus approximation of value functions and generalized Riccati equations*

Participants: Stéphane Gaubert, Zheng Qu, Shanjian Tang [Fudan University, Shanghai].

La thèse de Zheng Qu, supervisée par S. Gaubert et S. Tang, a porté sur le développement de méthodes tropicales en programmation dynamique approchée [12].

Les méthodes d'approximation max-plus conduisent à approcher la fonction valeur d'un problème de contrôle ou de jeux par un supremum d'un nombre fini de formes quadratiques, voir notamment [113]. On s'intéresse ici à l'analyse théorique (complexité) ainsi qu'à l'amélioration de ces méthodes. Dans certains cas, ces formes quadratiques sont propagées par des flots d'équations de Riccati généralisées. Afin d'effectuer des analyses d'erreur, on exploite les propriétés de contraction du flot de Riccati pour certaines métriques connues sur le cône des matrices positives, et en particulier pour la métrique de Thompson. Celle-ci n'est rien d'autre que $d_T(A,B) = \|\log \mathrm{spec}\,(A^{-1}B)\|_\infty$, où spec désigne la suite des valeurs propres d'une matrice, et log s'entend composante par composante.

Ceci nous a amené à étudier le problème général du calcul du taux de contraction d'un flot monotone sur un cône, pour la métrique de Thompson. En effet, les propriétés de contraction de l'équation de Riccati standard sont connues (résultats de Bougerol pour la métrique Riemanienne invariante, et de Wojtowski pour la métrique de Thompson), mais les techniques de preuve employées dans ce cadre (semigroupes de matrices symplectiques) ne s'étendent pas aux équations généralisées.

On donne dans [114], [28] une formule explicite générale pour le taux de contraction pour la métrique de Thompson d'un flot monotone, faisant seulement intervenir le générateur du flot et sa dérivée. On a notamment appliqué ce résultat à une équation de Riccati généralisée associé à des problèmes de contrôle stochastique avec critère quadratique, dans lesquels la dynamique comporte un terme bilinéaire en le contrôle et le bruit. On a montré dans ce cas que la métrique de Thompson est la seule métrique de Finsler invariante pour laquelle le flot est nonexpansif, et l'on a caractérisé la constante de contraction locale.

Une application de ces résultats à l'analyse d'une méthode de réduction de la malédiction de la dimension, dûe à McEneaney, a été donnée dans [28], [50].

English version

The PhD work of Zheng Qu, supervised by S. Gaubert and S. Tang, dealt with the development of tropical methods in approximate dynamic programming [12].

The max-plus methods lead to approach the value function of an optimal control or zero-sum game problem by a supremum of a finite number of quadratic forms, see in particular [113]. We are interested here in the theoretical analysis (complexity) of this class of methods, as well as of their improvement. In certain cases, the quadratic forms are propagated by the flows of generalized Riccati equations. In order to perform an error analysis, we need to use some contraction properties of the Riccati flow, for certain known metrics on the space of positive matrices, like Thompson's metric. The latter is nothing but $d_T(A,B) = \|\log \mathrm{spec}\,(A^{-1}B)\|_\infty$, where spec denotes the sequence of eigenvalues of a matrix, and log is understood entrywise.

This led us to study the general problem of computing the contraction rate of an order-preserving flow on a cone, with respect to Thompson's metric. Indeed, the contraction properties of the standard Riccati flow are known (theorem of Bougerol for the invariant Riemanian metric, of Wojtowski for the Thompson's metric), but the proof of these properties (based on symplectic semigroups) does not carry over to generalized Riccati equations.

We gave in [114],[28] a general explicit formula for the contraction rate with respect to Thompson's metric of an order-preserving flow, involving only the generator of the flow and its derivative. We applied in particular this result to a generalized Riccati equation, associated to stochastic optimal control problems with a quadratic cost and a bilinear dynamics (presence of a bilinear term between the control and the noise). We showed that in this case, the Thompson's metric is the only invariant Finsler metric in which the generalized Riccati flow is nonexpansive, and we characterized the local contraction rate of this flow.

Z. Qu has applied these results in [28], [50] to the analysis of a method of reduction of the curse of dimensionality, introduced by McEneaney.

6.4.5. Points fixes d'applications monotones homogènes et jeux à somme nulle/Fixed points of order preserving homogeneous maps and zero-sum games

Participants: Marianne Akian, Stéphane Gaubert, Antoine Hochart.

Les opérateurs de Shapley sont les opérateur de programmation dynamique pour des jeux à somme nulle, ce sont précisément les opérateurs qui préservent l'ordre et commutent avec l'addition d'une constante. Le travail de M2 d'Antoine Hochart a traité d'une sous-classe d'opérateurs de Shapley, qui commutent en outre avec la multiplication par une constante positive. Nous les appellerons ici *sans-paiement*, car ils apparaissent dans des classes de jeux où les paiements instantanés sont nuls - le paiement a lieu seulement le dernier jour (*recursive games*). Ils apparaissent aussi dans l'étude structurelle de familles paramétriques de jeux répétés avec espace d'état fini et information parfaite, si l'on suppose par exemple que les probabilités de transitions sont fixées, mais que les paiements sont des paramètres. À toute famille paramétrique de jeux est associée un opérateur sans paiements et les points fixes de ce dernier sont précisément les vecteurs de paiement moyen réalisables. Un problème de base consiste à vérifier si un opérateur sans paiement n'a que des points fixes triviaux (réduits à des multiples du vecteur unité), et si possible, de déterminer des caractéristiques plus précises de l'ensemble des points-fixes, par exemple, savoir s'il existe un point fixe d'argmin donné. Le premier problème est connu être co-NP-complet, même pour des jeux déterministes. Nous montrons cependant que le second problème (point fixe d'argming prescrit) peut être résolu en temps polynomial. La preuve repose sur la construction d'une correspondance de Galois entre les faces d'un hypercube qui sont invariantes par l'opérateur, ainsi que sur une réduction à un problème d'accessibilité dans un hypergraphe orienté.

English version

Shapley operators are the dynamic programming operators of zero-sum stochastic games, they can be characterized as order preserving maps commuting with the addition of a constant. The M2 work of Antoine Hochart has dealt with a subclass of Shapley operators which are characterized by the property of commuting with the multiplication by a positive constant. We call them *payment-free*, as they arise in the study of *recursive games*, in which the payment only occurs when the game stops. They also arise in the study of structural properties of parametric mean payoff games (the transition probabilities are fixed, not the transition payoffs) with finite action spaces and perfect information: their fixed point set can be shown to give all the possible mean payoff vectors of such games. A basic problem is to check whether the fixed point set of such an operator is trivial (reduced to the multiples of the unit vector), and more precisely to determine its characteristics, for instance decide whether there is a fixed point with a prescribed argmin. The former problem is already known to be co-NP-complete, even for deterministic games. We showed however that the latter can be solved in polynomial time. The proof relies on the construction of a Galois connection between faces of the hypercube that are invariant by the operator, and on a reduction to a reachability problem in a directed hypergraph.

6.5. Applications

6.5.1. Introduction

Nous présentons maintenant plusieurs travaux de nature appliquée, touchant à des domaines variés, dans lesquels nous exploitons certaines des techniques mathématiques présentées précédemment, et particulièrement celles qui relèvent de la théorie de Perron-Frobenius non-linéaire et de la convexité tropicale. Ces applications utilisent aussi des techniques d'algèbre linéaire ou d'optimisation convexe.

English version

In this section, we describe several applied works in which we use some of the theoretical tools developed by the team, including non-linear Perron-Frobenius theory and tropical convexity. Some of these applications also make an intensive use of linear algebraic and convex programming methods.

6.5.2. Propriétés des valeurs propres de Perron et de Floquet, et application en chronothérapeutique/Properties of Perron and Floquet eigenvalue, with an application to chronotherapeutics

Participants: Frédérique Billy [Projet BANG, Inria], Jean Clairambault [Projet BANG, Inria], Olivier Fercoq, Stéphane Gaubert, Thomas Lepoutre [Projet BANG puis DRACULA, Inria].

On s'intéresse à des modèles de systèmes dynamiques monotones structurés en âge représentant la croissance de populations de cellules (saines ou tumorales), à la suite de travaux de Clairambault et Perthame. Il s'agit de comprendre l'influence du contrôle circardien sur la croissance des cellules. Dans le cas stationnaire, le taux de croissance est représenté par une valeur propre de Perron. Dans le cas périodique, il s'agit d'une valeur propre de Floquet. Les travaux [39], [73], [72] portent sur l'identification de ces modèles ainsi que sur un problème de contrôle thérapeutique, consistant à minimiser le taux de croissance des cellules tumorales sous une contrainte de non-toxicité du traitement (maintien d'une population de cellules saines). Ce travail s'appuie en particulier sur un algorithme d'optimisation de la valeur propre de Perron d'une matrice développé par Fercoq dans un autre contexte [104].

Un développement récent de ce travail peut être trouvé dans [39]. Un travail théorique sur ce type de modèles est présenté dans [46].

English version

We study monotone dynamical systems representing the growth of cells (healthy or tumoral), following a work of Clairambault and Perthame. The goal is to understand how the circadian control influences the growth of cells. In the case of stationnary monotone systems, this growth is measured by the Perron root. In the time periodic case, this Perron root is replaced by a Floquet multiplier.

The works [39], [73], [72] deal with the identification of these models, together with a therapeutic control problem, consisting in minimizing the growth rate of tumoral cells, under a non-toxicity constraint (preserving the population of healthy cells). This works relies in particular on a fast algorithm to optimize the Perron eigenvalue of a matrix, developed by Fercoq in a different context [104].

A recent development of this work can be found in [39]. A theoretical work on this kind of models has been presented in [46].

6.5.3. Preuve formelle d'inégalités non-linéaires/Formal proofs of non-linear inequalities

Participants: Xavier Allamigeon, Stéphane Gaubert, Victor Magron, Benjamin Werner [LIX].

La thèse de Victor Magron [11], dirigée par Benjamin Werner, codirigée par Stéphane Gaubert et Xavier Allamigeon, a porté sur la certification de bornes inférieures de fonctions multivariées à valeurs réelles, définies par des expressions semi-algébriques ou transcendantes, et sur la preuve de validité de celles-ci au moyen de certificats dans l'assistant de preuves Coq.

De nombreuses inégalités de cette nature apparaissent notamment dans la preuve par Thomas Hales de la conjecture de Kepler. Voici un exemple typique d'inégalité à prouver.

LEMME 9922699028 FLYSPECK. *Soit K, $\Delta\mathbf{x}$, l, t et f définis comme suit:*

$$\begin{aligned}
K &:= [4, 6.3504]^3 \times [6.3504, 8] \times [4, 6.3504]^2 \ , \\
\Delta\mathbf{x} &:= x_1x_4(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) \\
&\quad + x_2x_5(x_1 - x_2 + x_3 + x_4 - x_5 + x_6) \\
&\quad + x_3x_6(x_1 + x_2 - x_3 + x_4 + x_5 - x_6) \\
&\quad - x_2x_3x_4 - x_1x_3x_5 - x_1x_2x_6 - x_4x_5x_6 \ , \\
l(\mathbf{x}) &:= -\pi/2 + 1.6294 - 0.2213(\sqrt{x_2} + \sqrt{x_3} + \sqrt{x_5} + \sqrt{x_6} - 8.0) \\
&\quad + 0.913(\sqrt{x_4} - 2.52) + 0.728(\sqrt{x_1} - 2.0) \ , \\
t(\mathbf{x}) &:= \arctan \tfrac{\partial_4 \Delta\mathbf{x}}{\sqrt{4x_1\Delta\mathbf{x}}} \ , \\
f(\mathbf{x}) &:= l(\mathbf{x}) + t(\mathbf{x}) \ .
\end{aligned}$$

Alors, $\forall \mathbf{x} \in K, f(\mathbf{x}) \geq 0$.

On s'est donc intéressé à des fonctions non-linéaires, faisant intervenir des opérations semi-algébriques ainsi que des fonctions transcendantes univariées ($\cos$, $\arctan$, $\exp$, etc).

De manière classique, on peut approcher les fonctions transcendantes qui interviennent de la sorte par des polynômes, ce qui permet de se ramener à des problèmes d'optimisation semi-algébriques, que l'on peut résoudre par des techniques de sommes de carrés creuses conduisant à des problèmes SDP. Cependant, en pratique, cette approche est limitée par la taille des SDP à résoudre, qui croît rapidement avec le degré des approximations polynomiales.

Dans ce travail de thèse, on a développé une méthode alternative, qui consiste a borner certains des constituants de la fonction non-linéaire par des suprema de formes quadratiques dont les Hessiens sont judicieusement choisis. On reprend donc ici l'idée des approximations "max-plus" initialement introduites en contrôle optimal, en s'appuyant sur des techniques d'interprétation abstraite (généralisation non-linéaire de la méthode des gabarits de Manna et al.). Ainsi, on obtient une nouvelle technique d'optimisation globale, basée sur les gabarits, qui exploite à la fois la precision des sommes de carrés et la capacité de passage à l'échelle des méthodes d'abstraction.

L'implémentation de ces méthodes d'approximation a abouti à un outil logiciel : `NLCertify`. Cet outil génère des certificats à partir d'approximations semi-algébriques et de sommes de carrés. Son interface avec Coq permet de bénéficier de l'arithmétique certifiée disponible dans l'assistant de preuves, et ainsi d'obtenir des estimateurs et des bornes valides pour chaque approximation.

Les performances de cet outil de certification ont été démontrées sur divers problèmes d'optimisation globale ainsi que sur des inégalités essentiellement serrées qui interviennent dans la preuve de Hales (projet Flyspeck).

Ce travail est exposé dans [25], [26].

English version

The PhD work of Victor Magron [11], supervised by Benjamin Werner, and cosupervised by Stéphane Gaubert and Xavier Allamigeon, dealt with the certification of lower bounds for multivariate functions, defined by semi-algebraic or transcendental expressions, and their correctness proof through certificates checked in the Coq proof assistant.

Many inequalities of this kind appear in particular in the proof by Thomas Hales of Kepler's conjecture. Here is a typical example of inequality.

LEMMA 9922699028 FLYSPECK. *Let K, $\Delta\mathbf{x}$, l, t and f be defined as follows:*

$$\begin{aligned}
K &:= [4, 6.3504]^3 \times [6.3504, 8] \times [4, 6.3504]^2 \ , \\
\Delta\mathbf{x} &:= x_1x_4(-x_1 + x_2 + x_3 - x_4 + x_5 + x_6) \\
&\quad + x_2x_5(x_1 - x_2 + x_3 + x_4 - x_5 + x_6) \\
&\quad + x_3x_6(x_1 + x_2 - x_3 + x_4 + x_5 - x_6) \\
&\quad - x_2x_3x_4 - x_1x_3x_5 - x_1x_2x_6 - x_4x_5x_6 \ , \\
l(\mathbf{x}) &:= -\pi/2 + 1.6294 - 0.2213(\sqrt{x_2} + \sqrt{x_3} + \sqrt{x_5} + \sqrt{x_6} - 8.0) \\
&\quad + 0.913(\sqrt{x_4} - 2.52) + 0.728(\sqrt{x_1} - 2.0) \ , \\
t(\mathbf{x}) &:= \arctan \tfrac{\partial_4 \Delta\mathbf{x}}{\sqrt{4x_1 \Delta\mathbf{x}}} \ , \\
f(\mathbf{x}) &:= l(\mathbf{x}) + t(\mathbf{x}) \ .
\end{aligned}$$

Then, $\forall \mathbf{x} \in K, f(\mathbf{x}) \geq 0$.

Thus, we considered non-linear functions, defined in terms of semi-algebraic operations and univariate transcendental functions ($\cos$, $\arctan$, $\exp$, etc).

Such transcendental functions can be classically approximated by polynomials, which leads to semi-algebraic optimization problems, which can be solved by sparse sum of squares techniques leading to SDP formulations. However, in practice, this approach is limited by the growth of the size of the SDP instances to be solved, whichs grows quickly with the degree of polynomial approximations.

In this PhD, we developed an alternative method, which consists in bounding some constituents of the non-linear function to be optimized by suprema of quadratic forms with well chosen Hessians. This is based on the idea of "maxplus approximation" initially introduced in optimal control, and also, on abstract interpretation (the template method introduced by Manna et al. in static analysis). In this way, we end up with a new global optimization technique, which takes advantage of the precision of sum of squares and of the scalability of abstraction methods.

These methods have been implemented in a software tool: `NLCertify`. This tool generates certificates from semi-algebraic and sum of square certificates. Its interface with Coq allows one to take benefit of the certified arithmetics available in this proof assistant, and so, to obtain estimators and valid bounds for each approximation.

The performances of this certification tool have been shown on several global optimization problems from the litterature, as well as on essentially tight inequalities taken from Hales' proof (Flyspeck project).

This work is presented in [25], [26].

6.5.4. *Vérification de systèmes temps-réels/Verification of real-time systems*

Participants: Xavier Allamigeon, Uli Fahrenberg [IRISA], Stéphane Gaubert, Ricardo Katz [Conicet], Axel Legay [IRISA].

Dans [141], Lu, Madsen, Milata, Ravn, Fahrenberg et Larsen ont montré que les polyèdres tropicaux peuvent être utilisés dans le cadre de l'analyse d'accessibilité d'automates temporisés. En effet, les polyèdres tropicaux expriment naturellement des invariants non-convexes, qui sont en fait des disjonctions d'invariants fournis par des DBM (*difference bound matrices*). A ce titre, les polyèdres tropicaux devraient permettre de réduire le nombre de disjonctions réalisées pendant l'analyse d'automates temporisés. Une limitation importante de cette approche est cependant que les polyèdres tropicaux sont topologiquement fermés, et qu'ils ne peuvent donc pas exprimer de contraintes d'inégalités strictes. Ces dernières sont néanmoins fondamentales dans l'analyse de systèmes temps-réels.

Nous avons donc développé dans [44] une généralisation des polyèdres tropicaux permettant d'exprimer des contraintes mixtes, *i.e.* strictes ou larges. Notre approche repose sur l'utilisation d'inégalités tropicales linéaires à coefficients dans un (quotient du) semi-anneau de germes affines. Afin de réaliser des opérations sur cette nouvelle classe de polyèdres tropicaux, nous avons défini deux nouveaux algorithmes. Le premier est un analogue tropical de l'élimination de Fourier-Motzkin. Celle-ci s'applique plus généralement à des systèmes d'inégalités linéaires sur des semi-anneaux idempotents et totalement ordonnés. Le second algorithme permet de tester si un système de contraintes mixtes admet une solution. Nous montrons en effet que ce problème est équivalent en temps polynomial à la résolution d'un problème de jeux déterministes à somme nulle. Ces deux contributions nous permettent de définir les primitives requises pour l'analyse d'accessibilité d'automates temporisés.

English version

Lu, Madsen, Milata, Ravn, Fahrenberg and Larsen have shown in [141] that tropical polyhedra can be applied to the reachability analysis of timed automata. Indeed, tropical polyhedra naturally express non-convex invariants, which correspond to disjunctions of invariants provided by DBM (*difference bound matrices*). Consequently, tropical polyhedra should allow to reduce the number of disjunctions arising during the analysis of timed automata. An important limitation of this approach is that tropical polyhedra are topologically closed, and thus they cannot express strict inequality constraints. However, such constraints plays an important role in the analysis of real-time systems.

As a result, we have developed in [44] a generalization of tropical polyhedra, in order to express mixed constraints, *i.e.* strict or loose ones. Our approach relies on tropical linear inequalities with coefficients in a (quotient of) the semiring of affine germs. In order to perform operations on this new class of polyhedra, we have introduced two new algorithms. The first one is a tropical analog of Fourier-Moztkin elimination. In fact, it applies more generally to systems of linear inequalities over totally ordered and idempotent semirings. The second algorithm allows to test the feasability of a mixed constraint system. We indeed show that this problem is polynomial-time equivalent to solving mean payoff games. These two contributions allow to define the primitives required by the reachability analysis of timed automata.

MCTAO Project-Team

6. New Results

6.1. Optimal control for quantum systems: the contrast problem in NMR

These studies aim at optimizing the contrast in Nuclear Magnetic Resonance imaging using advanced optimal control. As said in section 4.2 , our work on this problem is based on experiments conducted in Prof. S. Glaser in Munich, see [29].

6.1.1. Theoretical aspects

Participants: Bernard Bonnard, John Marriott, Monique Chyba [University of Hawaii], Gautier Picot [University of Hawaii], Olivier Cots, Jean-Baptiste Caillau.

This is done in collaboration with University of Hawaii, and deals with many theoretical aspects of the contrast problem in NMR: analysis of the optimal flow [5], feedback classification in relation with the relaxation times of the species [10], [4]. John Marriott defended his PhD thesis on this topic, on August 28, 2013.

6.1.2. Numerical aspects

Participants: Bernard Bonnard, Jean-Baptiste Caillau, Olivier Cots, Mathieu Claeys [LAAS CNRS, Toulouse], Pierre Martinon [COMMANDS team, Inria].

We performed, in a collaboration with Pierre Martinon (COMMANDS team, Inria) and Mathieu Claeys (LAAS CNRS, Toulouse), a thorough comparison of the various available numerical methods in optimal control on this important physical problem. Direct and indirect methods (implemented in the Bocop and Hampath sofwares) were tested in the contrast problem, and LMI techniques were used to obtain global bounds on the extremum (in the contrast problem there are many local optima and the global optimality is a complicated issue). This successful collaboration is accounted for in [15] and was presented at the CDC conference [12]

6.2. Conjugate and cut loci computations and applications

Participants: Bernard Bonnard, Olivier Cots, Jean-Baptiste Caillau.

One of the most important results obtained by B. Bonnard and his collaborators concern the explicit computations of conjugate and cut loci on surfaces. This has obvious applications in optimal control to compute the global optimum; it is also relevent in optimal transport where regularity properties of the transport map in the Monge problem is related to convexity properties of the tangent injectivity domains.

In [3], we complete the previous results obtained in [27] (we bring them from ellipsoids to general revolutions surfaces).

The conjugate and cut loci in Serret-Andoyer metrics and dynamics of spin particles with Ising coupling are analized in [7], this is a first step towards the computation of conjugate and cut loci on left invariant Riemannian and sub Riemannian metrics in S0(3) with applications for instance to the attitude control problem of a spacecraft.

An analysis of *singular* metrics on revolution surfaces, motivated by the average orbital transfer problem when the thrust direction is restricted, is proposed in [2].

Finally, [8] determines cut and conjugate loci in an enegy minimizing problem that is related to the quantum systems mentionned in the first paragraph of section 4.2 .

6.3. Averaging in control

Participants: Bernard Bonnard, Helen-Clare Henninger, Jean-Baptiste Pomet.

A paper on the construction and properties of an "average control system" [1] appeared this year, it is based on Alex Bombrun's doctoral work (2007). It connects solutions of highly oscillating control systems to those of an average control system, when the frequency of oscillation goes high. It also gives a better ground to averaging for minimum time.

This average system in the case of minimum time for low thrust orbit transfer in the two body problem is currently being explored, in particular the study of its inherent singularities. In [16] we give some properties of this system, like geodesic convexity, and compare it with the one obtained for minimum energy, and Helen Henninger's PhD aims at going further in this direction and then apply this local study to real missions, possibly in a three-body environment.

6.4. Optimal transport

Participants: Ludovic Rifford, Alice Erlinger, Alessio Figalli [U. of Texas at Austin, USA], Thomas Gallouet [Inria, SIMPAF team], Bernard Bonnard, Jean-Baptiste Caillau, Lionel Jassionesse, Robert Mc Cann [U. of Toronto].

- The very general condition for continuity of the transport map given in [41] motivated exploration of conditions for convexity of the tangent injectivity domain [42], [3]. Lionel Jassionnesse's PhD is in part devoted to Ma-Trudinger-Wang tensor that also plays an important role in this matter. Ludovic Rifford has an ongoing collaboration with Alession Figalli and Thomas Gallouet on the link between this MTW tansor and the convexity of injectivity domains; They already improved a result by Loeper and Villani (the preprint "Ma-Trudinger-Wang condition vs. convexity of injectivity domains" is available from the authors) and aim at proving a conjecture due to Villani, that would hold in the case of anlaytic surfaces.
- The goal of Alice Erlinger's PhD, joint with University of Toronto, is to explore Optimal Transport's application to modeling in economics. She unfortunately stopped her PhD, but some results have already been obtained.

6.5. Applications of control methods to dynamical systems

Participants: Gonzalo Contreras, Alessio Figalli, Ayadi Lazrag, Ludovic Rifford, Raffael Ruggiero.

Ludovic Rifford and collaborators have been applying with success, techniques from geometric control theory to open problems in dynamical systems, mostly on genericity properties and using controllability methods to build suitable perturbations.

This has been applied to closing geodesics [64]. Ayadi Lazrag's PhD also deals with such problems; applying techniques close to these in [65], one goal is to establish a version of Francks' lemma for geodesic flows and to apply this to persitence problems. The approach relies on control theory results, with order 2 conditions. See [18] and another preprint ("Franks' lemma for C^2-Mañé perturbations of Riemannian metrics and applications to persistence" by Lazrag, Rifford and Ruggiero, available from the authors).

In [17], a non trivial conjecture on generic hyperbolicity of the so-called Aubry set of a Hamiltonian is solved on compact surfaces and in the C^2 topology (for genericity).

NECS Project-Team

6. New Results

6.1. Networked systems and graph analysis

6.1.1. Distributed graph-discovery

Participants: A. Kibangou [Contact person], T.-M. D. Tran, F. Garin, A. de Almeida [UFC Brazil].

The availability of information on the communication topology of a wireless sensor network is essential for the design of the estimation algorithms. In the context of distributed self-organized sensor networks, there is no central unit with the knowledge of the network, and the agents must run some distributed network discovery algorithm.

We have studied the problem of estimating the eigenvalues of the Laplacian matrix associated with a graph modeling the interconnections between the nodes of a given network. Our approach is based on properties resulting from the factorization of the average consensus matrix. Indeed, as recently shown [45], the average consensus matrix can be written as a product of Laplacian based consensus matrices whose stepsizes are given by the inverse of the nonzero Laplacian eigenvalues. By distributively solving the factorization of the average consensus matrix, we have shown that the Laplacian eigenvalues can be computed as the inverse of the stepsizes in each estimated factor, where these factors are constrained to be structured as Laplacian based consensus matrices. A constrained optimization problem was formulated and distributed gradient descent methods have been formulated. As formulated, the problem can be viewed as a consensus problem with equality constraints. In contrast to the state-of-the-art, the proposed algorithm does not require great resources in both computation and storage. This algorithm can also be viewed as a way for decentralizing the design of finite-time average consensus protocol recently proposed in the literature.

Laplacian eigenvalues have several interesting properties that can help to study networks, however they cannot uniquely characterize the topology of the network. Therefore, we have directly studied the problem of topology identification in [20]. The considered set-up concerns a collaborative wireless sensor network where nodes locally exchange coded informative data before transmitting the combined data towards a remote fusion center equipped with an antenna array. For this communication scenario, a new blind estimation algorithm was developed for jointly recovering network transmitted data and connection topology at the fusion center. The proposed algorithm is based on a two-stage approach. The first stage is concerned with the estimation of the channel gains linking the nodes to the fusion center antennas. The second stage performs a joint estimation of network data and connection topology matrices by exploiting a constrained (PARALIND) tensor model for the collected data at the fusion center.

Distributed network-discovery algorithms become even more challenging in the case where the algorithm must be anonymous, namely in the case when the agents do not have or do not want to disclose their identifiers (id.s), either for technological reasons (in time-varying self-organized networks, assigning unique identifiers to agents is a challenge) or for privacy concerns. In anonymous networks, even simple tasks such as counting the number of agents are challenging problems. In [24] we have proposed an algorithm for node-counting in anoymous networks. It is based on a graph-constrained LTI system similar to linear consensus, and on system identification: the idea is that the order of the system is the number of agents, and based on local observations each agent tries to identify the order of the system, testing the rank of the Hankel matrix from the output data.

6.1.2. Observability in consensus networks

Participants: A. Kibangou [Contact person], C. Commault [Grenoble INP].

Studying the observability problem of a system consists in answering the question: is it possible, for a given node, to reconstruct the entire network state just from its own measurements and those of its neighbors? Studying observability for arbitrary graphs is particularly a tough task, therefore, studies are generally restricted to some families of graphs; for instance, recently, observability has been studied for paths and circular graphs and also grids where the study was carried out based on rules on number theory. We have considered families of graphs admitting an association scheme such that strongly regular graphs and distance regular graphs. The regularity properties of these kinds of graphs can particularly be useful for robustifying the network as for cryptographic systems. Based on the so-called Bose-Mesner algebra, we have stated observability conditions on consensus networks modeled with graphs modeled with strongly regular graphs and distance regular graphs; for this purpose, we have introduced the notion of local observability bipartite graph that allows characterizing the observability in consensus networks. We have shown that the observability condition is given by the nullity of the so-called "local bipartite observability graph"; when the nullity of the graph cannot be derived directly from the structure of the local bipartite observability graph, the rank of the associated bi-adjacency matrix allows evaluating the observability. The bi-adjacency matrix of the local bipartite observability graph must be full column rank for guaranteeing observability. From this general necessary and sufficient condition, we have deduced sufficient conditions for strongly regular graphs and distance regular graphs [25].

6.2. Collaborative and distributed algorithms

6.2.1. Finite-time average consensus

Participants: A. Kibangou [Contact person], T.-M. D. Tran.

Nowadays, several distributed estimation algorithms are based on the average consensus concept. Average consensus can be reached using a linear iterations scheme where each node repeatedly updates its value as a weighted linear combination of its own value and those of its neighbors; the main benefit of using a linear iterations scheme is that, at each time-step, each node only has to transmit a single value to each of its neighbors. Based on such a scheme, several algorithms have been proposed in the literature; however, in the most proposed algorithms the weights are chosen so that all the nodes asymptotically converge to the same value. Sometimes, consensus can be embedded as a step of more sophisticated distributed; obviously, asymptotic convergence is not suitable for these kinds of distributed methods, and therefore it is interesting to address the question of exact consensus in finite-time. For time-invariant network topologies and in the perfect information exchange case, i.e., without channel noise nor quantization, we have shown that the finite-time average consensus problem can be solved as a matrix factorization problem with joint diagonalizable matrices depending on the graph Laplacian eigenvalues; moreover, the number of iterations is equal to the number of distinct nonzero eigenvalues of the graph Laplacian matrix. The design of such a protocol requires the knowledge of the Laplacian spectrum, which can be carried out in a distributed way (see Section 6.1.1 . The matrix factorization problem is solved in a distributed way, in particular a learning method was proposed and the optimization problem was solved by means of distributed gradient backpropagation algorithms. The factor matrices are not necessarily symmetric and the number of these factor matrices is exactly equal to the diameter of the graph [30].

6.2.2. Linear consensus in large-scale geometric graphs

Participants: F. Garin [Contact person], E. Lovisari [Lund], S. Zampieri [Padova].

Traditional analysis of linear average-consensus algorithms studies, for a given communication graph, the convergence rate, given by the essential spectral radius of the transition matrix (i.e., the second largest eigenvalues' modulus). For many graph families, such analysis predicts a performance which degrades when the number of agents grows, basically because spreading information across a larger graph requires a longer time; however, when considering other well-known quadratic performance indices (involving all the eigenvalues of the transition matrix), the scaling law with respect to the number of agents can be different. This is consistent with the fact that, in many applications, for example in estimation problems, it is natural to expect that a larger number of cooperating agents has a positive, not a negative effect on performance. It is

natural to use a different performance measure when the algorithm is used for different purposes, e.g., within a distributed estimation or control algorithm. We are interested in evaluating the effect of the topology of the communication graph on performance, in particular for large-scale graphs. We have focused on graph families which can describe sensor networks, and hence have geometric constraints, namely nodes can be connected only with nearby nodes in the sense of Euclidean distance [16].

6.2.3. Distributed computation methods for multidimensional data

Participants: A. Kibangou [Contact person], A. de Almeida [UFC Brazil].

In [19], we consider the issue of distributed computation of tensor decompositions. A central unit observing a global data tensor assigns different data sub-tensors to several computing nodes grouped into clusters. The goal is to distribute the computation of a tensor decomposition across the different computing nodes of the network, which is particularly useful when dealing with large-scale data tensors. However, this is only possible when the data sub-tensors assigned to each computing node in a cluster satisfies minimum conditions for uniqueness. By allowing collaboration between computing nodes in a cluster, we show that average consensus based estimation is useful to yield unique estimates of the factor matrices of each data sub-tensor. Moreover, an essentially unique reconstruction of the global factor matrices at the central unit is possible by allowing the subtensors assigned to different clusters to overlap in one or several modes. The proposed approach is useful to a number of distributed tensor-based estimation problems in signal and data processing.

6.2.4. Collaborative source seeking

Participants: C. Canudas de Wit [Contact person], R. Fabbiano, F. Garin, Y. Gaudfrin, J. Dumon.

The problem of source localization consists in finding, with one or several agents possibly cooperating with each other, the point or the spatial region from which a quantity of interest is being emitted. Source-seeking agents can be fixed sensors, that collect and exchange some information about the signal field and try to identify the position of the source (or the smallest region in which it is included), or moving devices equipped with one or more sensors, that physically reach the source in an individual or cooperative way. This research area is attracting a rapidly increasing interest, in particular in applications where the agents have limited or no position information and GPS navigation is not available, as in underwater navigation or in cave exploration: for instance, source localization is relevant to many applications of vapor emitting sources such as explosive detection, drug detection, sensing leakage or hazardous chemicals, pollution sensing and environmental studies. Other fields of interest are sound source localization, heat source localization and vent sources in underwater field. Techniques present in literature either are based on a specific knowledge of the solution of the diffusion process, or make use of an extremum-seeking approach, exciting the system with a periodic signal so as to explore the field and collect enough information to reconstruct the gradient of the quantity of interest. Our approach lies in the computation of derivatives (potentially of any order) from Poisson integrals that, for isotropic diffusive source in steady-state, whose solution satisfies the Laplace equation, allows for a gradient search with a small computation load (derivatives are computed by integrals) and without requiring any knowledge of the closed-form solution, avoiding in the same time extremum-seeking oscillations; this has the additional advantage of an intrinsic high-frequency filtering, that makes the method low sensitive to measurement noise. This work is the topic of the Ph.D. of Ruggero Fabbiano, and is described in papers under review.

Moreover, a hardware implementation of the source-seeking algorithm has been done during the internship of Yvan Gaudfrin, at GIPSA-LAB with the support of Jonathan Dumon. A description of the setup and videos of the source-seeking robot are available online: http://necs.inrialpes.fr/pages/platforms.php

6.3. Sensor networks: estimation and data fusion

6.3.1. Data fusion approaches for motion capture by inertial and magnetic sensors

Participants: H. Fourati [Contact person], A. Makni, A. Kibangou.

We are interested to motion capture (or attitude) by fusing Inertial and Magnetic Sensors. In [15], we present a viable quaternion-based Complementary Observer (CO) which is designed for rigid body attitude estimation. The CO processes data from a small inertial/magnetic sensor module containing tri-axial angular rate sensors, accelerometers, and magnetometers, without resorting to GPS data. The proposed algorithm incorporates a motion kinematic model and adopts a two-layer filter architecture. In the latter, the Levenberg Marquardt Algorithm (LMA) pre-processes acceleration and local magnetic field measurements, to produce what will be called the system's output. The system's output together with the angular rate measurements will become measurement signals for the CO. In this way, the overall CO design is greatly simplified. The efficiency of the CO is experimentally investigated through an industrial robot and a commercial IMU during human segment motion exercises. In a recent work [35], a viable quaternion-based Adaptive Kalman Filter (q-AKF) that is designed for rigid body attitude estimation. This approach is an alternative to overcome the limitations of the classical Kalman filter. The q-AKF processes data from a small inertial/magnetic sensor module containing triaxial gyroscopes, accelerometers, and magnetometers. The proposed approach addresses two challenges. The first one concerns attitude estimation during various dynamic conditions, in which external acceleration occurs. Although external acceleration is one of the main source of loss of performance in attitude estimation methods, this problem has not been sufficiently addressed in the literature. An adaptive algorithm compensating external acceleration from the residual in the accelerometer is proposed. At each step, the covariance matrix associated with the external acceleration is estimated to adaptively tune the filter gain. The second challenge is focused on the energy consumption issue of gyroscopes for long-term battery life of Inertial Measurement Units. We study the way to reduce the gyro measurement acquisition while maintaining acceptable attitude estimation. Through numerical simulations, under external acceleration and parsimonious gyroscope's use, the efficiency of the proposed q-AKF is illustrated.

6.3.2. Pedestrian dead-reckoning navigation

Participant: H. Fourati [Contact person].

We proposes a foot-mounted Zero Velocity Update (ZVU) aided Inertial Measurement Unit (IMU) filtering algorithm for pedestrian tracking in indoor environment [22]. The algorithm outputs are the foot kinematic parameters, which include foot orientation, position, velocity, acceleration, and gait phase. The foot motion filtering algorithm incorporates methods for orientation estimation, gait detection, and position estimation. A novel Complementary Filter (CF) is introduced to better pre-process the sensor data from a foot-mounted IMU containing tri-axial angular rate sensors, accelerometers, and magnetometers and to estimate the foot orientation without resorting to GPS data. A gait detection is accomplished using a simple states detector that transitions between states based on acceleration measurements [32]. Once foot orientation is computed, position estimates are obtained by using integrating acceleration and velocity data, which has been corrected at step stance phase for drift using an implemented ZVU algorithm, leading to a position accuracy improvement. We illustrate our findings experimentally by using of a commercial IMU during regular human walking trial in a typical public building. Experiment results show that the positioning approach achieves approximately a position accuracy less than 1 m and improves the performance regarding a previous work of literature [33].

6.3.3. Sensor placement of unreliable sensors

Participants: F. Garin [Contact person], P. Frasca [Twente].

In this work (see [23]), we consider problems in which sensors have to be deployed in a given environment in such a way to provide good coverage of it. It is clear that sensor failures may deteriorate the performance of the resulting sensor network. Then, it is also natural to ask if taking into account such uncertainties changes the coverage optimization problem and leads to a different optimal solution. For simplicity, we start considering a one-dimensional problem, where sensors are to be placed on a line in such a way to optimize the disk-coverage cost The optimal solution for reliable sensors is simply an equally-spaced configuration of the sensors. If we allow that the sensors may fail to take or communicate their measurements, this solution may instead not be optimal. However, as the number of sensors grows to infinity, the ratio between the cost of equally-spaced configurations and the optimal failure-free cost only grows as the logarithm of the number of sensors. We interpret this result as a confirmation of the intrinsic robustness of sensor networks.

6.4. Control design and co-design

6.4.1. Energy-aware networked control

Participants: C. Canudas de Wit [Contact person], F. Garin, N. Cardoso de Castro, D. Quevedo [Newcastle].

We have considered an event-based approach to energy-efficient management of the radio chip in the sensor node of a wireless networked control system. Indeed the radio is the main energy consumer, and intermittent data transmission allows one to reduce the use of the radio. While the existing literature in the control community on event-based control only addresses policies using two radio modes (transmitting/sleep), our work follows some considerations on the radio chip modes well-known in the communication networks literature, and introduces various radio-modes: different 'idle' non-transmitting modes, where only part of the radio chip is switched off (thus consuming more energy than 'sleep', but allowing for faster transition to transmission), and various transmitting modes, with different power levels. We propose an event-based radio-mode switching policy, which allows to perform a trade-off between energy saving and performance of the control application; to this end, a switched model describes the system, taking into account control and communication. The optimal switching policy is computed using dynamic programming, considering a cost either over an infinite time-horizon (see [31]) or over a finite receding horizon (joint work with D. Quevedo, Univ. Newcastle, Australia, described in a paper in preparation).

6.4.2. Adaptive control strategy based reference model for spacecraft motion trajectory

Participants: H. Fourati [Contact person], Z. Samigulina.

In aerospace field, the economic realization of a spacecraft is one of the main objectives which should be accomplished by conceiving the optimal propulsion system and the best control algorithms. Our work focuses on the development of a viable Adaptive Control Approach (ACA) for Spacecraft Motion Trajectory (SMT), see [39].The proposed strategy involves the nonlinear mathematical model of SMT expressed in the central field, which is linearized by the Taylor expansion, and the second Lyapunov method to offer a high rate and unfailing performance in the functioning. The adaptive control system is composed of the cascade of adaptation loop and feedback control loop. When the spacecraft deviates from its reference trajectory model, the ACA acts on the control system to correct this deviation and follow the optimal reference trajectory. Therefore, when the states of the adjustable model are different from its reference values, then the error signal is provided as an input to the adaptation law, which contains the adaptation algorithm. The output will be the state variable feedback control matrix which will be used to calculate the new control law vector. The efficiencies of the linearization procedure and the control approach are theoretically investigated through some realistic simulations and tests under MATLAB. The steady state errors of control between the reference model and the adjustable model of SMT converge to zero. This work is described in [38].

6.5. Transportation networks and vehicular systems

6.5.1. Traffic estimation and prediction

Participants: C. Canudas de Wit [Contact person], A. Kibangou, L. Leon Ojeda, F. Morbidi.

Reconstructing densities in portions of the road links not equipped with sensors constitutes an important task in traffic estimation, forecasting, and control problems. Among many other approaches, model-based observers is one popular technique to build this information. They can also be understood as *virtual sensors* deployed inside of the cells not equipped with *true sensors*. They are used to better track, in real-time, density variations with a fine degree of granularity in the space, as the *virtual cells* can be selected as small as desired.

In [43], a graph constrained-CTM observer was introduced. It allows reconstructing rather accurately the internal states (densities) of a road portion not equipped with sensors. This strategy for real-time density estimation was applied on Grenoble South Ring. In [27], this observer has been associated with an adaptive Kalman filtering approach for traffic prediction in terms of travel time. The adaptive Kalman filtering approach was also been used for predicting input flows in [26].

6.5.2. Traffic control

Participants: C. Canudas de Wit [Contact person], D. Pisarski.

This work has been conducted in two parallel directions, combining steady state analysis and design of an optimal ramp metering controller.

The first direction was to extend the preliminary results presented in the papers [10] and [46]. The goal was to implement the idea of optimal steady state balancing. A relevant software was built up and tested on the model representing the south ring of Grenoble. The results were published in [28]. A comprehensive study of steady state balancing was submitted as a journal paper, under review.

The second direction was to develop a distributed optimal ramp metering controller. This study is motivated by two following facts. The first one is to decentralize and parallelize computation for optimal freeway traffic control problem, and thus to reduce computational complexity. The second one is to reduce the lengths of the communication channels, in order to eliminate the probability of information delay or packet loss. The proposed new control objective provides a uniformly distributed (or balanced) vehicle density such that the usage of freeway (measured by the Total Travel Distance and Total Input Volume) is maximized. This optimal balancing objective is reached by taking a proper state feedback control structure and optimizing the set of gains. Here we imposed distributed condition for both, the feedback structure and the optimization process. We have focused the efforts to design the controller network architecture that is based on the common elements (ramp meter controllers), executing the same computational procedures and applying the control signals based on the same state-feedback structure. This meets a spirit of 'plug and play' (PnP), and is beneficial for both, architecture assembling and component replacement (in case of failure). In order to define the functionality for each of this PnP controller, the analysis on both system controllability and conditions for optimality were carried on. The preliminary work let us to determine the what type of information and upon which communication topology it is required to be sent in order to solve the posed optimization problem. Firstly, the feedback controls for each of the controllers require state information of the section that is controllable for it. In general, each of the controllers demands the state for its closest surrounding sections (downstream and upstream). Secondly, each of the controllers communicates with its closest active neighbors to exchange the information of optimal solution, namely optimal boundary flow or optimal control. We also observed that in any system mode there might be only one inactive controller (the controller that does not have any controllable section) surrounded by two active ones, and thus the maximum required information comes from the two closest neighbors for each of the directions. We noticed also that inactive controllers may serve to convey the information for the active ones, so the communication can be based on a path (or linear) graph. Part of this research was realized in UC Berkeley during the visit of Dominik Pisarski in PATH laboratory.

Traffic control is based on models of traffic, usually the so-called CTM – Cell transmission Model. Some work in the team aims at developing different models, more suitable for control. One such model is based on cells of variable length, as an alternative way to describe the congestion position. This model, proposed in [42], has been refined in the master thesis of Giulio Bontadini, taking into account mass conservation laws.

6.5.3. Vehicle control for disabled people

Participants: C. Canudas de Wit [Contact person], V. Ciarla, J. Dumon, F. Quaine [UJF], V. Cahouet [UJF].

Disabled people face the effort to turn the steering wheel while driving their vehicle. This study, funded by the VolHand project, focuses on the aspect of the assistance during driving maneuver at low speeds (for instance, parking). On common vehicles for healthy people, the system that improves the driver's steering feel in these situations is the power-steering stage, which is mounted at the basis of the steering column and is based on hydraulic technology; the new generation uses an electric motor instead of the hydraulic pump, with more advantages in terms of fuel consumption, better road-feel feedback to the driver and better return-to-center performances of the steering wheel. This work has developed a general methodology to adapt the current technology for disabled people, by introducing additional blocks that can be implemented via software without altering the hardware of the vehicle. In this way, it can be easily exported without additional costs in terms of design and technology for the industrial partner. The methodology has been studied theoretically, joining control aspects with bio-mechanical ones. Moreover, the theoretical study has been tested in laboratory on the

hardware-in-the loop setup, using the experimental platform NeCSCar (see Section 5.2). First, a real steering wheel has been linked to a real-time PC-unit and to an electrical motor. A graphical user interface has been implemented to facilitate the access to the software. Then, the last part of the study has been the experimental validation with a tele-operated real vehicle. The vehicle provided the measure of the friction torque to the PC-unit, simulating a real driving situation.

This work is described in [41] and in the Ph.D. thesis [11].

6.5.4. Control of communicating vehicles in urban environment

Participants: C. Canudas de Wit [Contact person], G. de Nunzio.

For a given vehicle there are different ways to travel on a given distance in a given time, associated to different levels of energy consumption; therefore, it is always possible to find an energy-optimal trajectory. Advising the driver via a suitable interface can reduce the energy consumed during the travel, and thus improve the energy efficiency: this is the principle of eco-driving. In urban areas, the optimal trajectory of the vehicle depends on interactions with other vehicles, also on passive signs (panels, priorities, etc.) and active signs (traffic lights); in each case, constraints are imposed on the command (vehicle speed). From the infrastructure perspective, traffic control in urban areas consists in determining the state of traffic signals in order to solve an optimization problem, for example minimizing average travel time of vehicles in the road network. If all vehicles could communicate with one another and with the active infrastructure (traffic lights), we could imagine benefits for each of the two problems which can be considered as a whole: on the one hand, from the vehicles' point of view, more information is available that can be integrated into the online optimization problem; on the other hand, there are new measures and new commands available to control traffic. Indeed, the estimation of the traffic is no longer necessary, as the position and speed of approaching vehicles is known and shared. More importantly, the traffic manager can send instructions to the vehicles. The aim of the research is to evaluate the potential in terms of energy saving and traffic improvement made possible by communicating vehicles. This work is the topic of the Ph.D. thesis of Giovanni De Nunzio, a CIFRE thesis with IFPEN. The paper [21] considers the scenario where vehicle and infrastructure (traffic lights) can communicate, and describes a suitable optimization algorithm that can be run on-board the vehicle so to optimize its energy consumption by avoiding stops and abrupt changes of speed at traffic lights, thanks to the information on upcoming traffic lights on the same road.

NON-A Project-Team

6. New Results

6.1. Homogeneity theory and analysis of nonlinear systems

Homogeneity is a kind of symmetry, if it is presented in a system model, then it may simplify analysis of stability and performance properties of the system. The new results obtained in 2013 are as follows:

- The notion of geometric homogeneity has been extended for differential inclusions in [44]. This kind of homogeneity provides the most advanced coordinate-free framework for analysis and synthesis of nonlinear discontinuous systems. Theorem of L. Rosier on a homogeneous Lyapunov function existence and an equivalent notion of global asymptotic stability for differential inclusions have been presented. Robustness properties (ISS) of sliding mode systems applying the homogeneity concept have been considered in [46].
- Retraction obstruction for time-varying stabilization on compact manifolds has been revisited in [13].
- Several conditions have been proposed to check different robustness properties (ISS, iISS, IOSS and OSS) for generic nonlinear systems applying the weighted homogeneity concept (global or local) in [14], [45]. The advantages of this result are that, under some mild conditions, the system robustness can be established as a function of the degree of homogeneity.
- A new algorithm for the analysis of strange attractors has been presented in [51]. An application of that results for observability-singularity manifolds in the context of chaos based cryptography has been given in [52].
- Exciting multi-DOF systems by feedback resonance has been considered in [20].
- Some conditions on existence of oscillations in hybrid systems have been established in [23], [57]. An application to a humanoid robot locomotion has been considered.
- Considering two chaotic Rossler systems, the paper [83] presents a study on the forced synchronization of two systems, bidirectionally coupled by transmitting unidirectional signals which explicitly depend on a single state variable (from the emitter) and only affect directly the dynamics corresponding to the transmitted state variable (of the receiver).
- The paper [33] is concerned with the construction of local observers for nonlinear systems without inputs, satisfying an observability rank condition. The aim of this study is, first, to define a homogeneous approximation that keeps the observability property unchanged. This approximation is further used in the synthesis of local observer which is proven to be locally convergent for Lyapunov-stable systems.
- The paper [74] addresses the problem of exact average-consensus reaching in a prescribed time. The communication topology is assumed to be defined by a weighted undirected graph and the agents are represented by integrators. A nonlinear control protocol, which ensures a finite-time convergence, is proposed. With the designed protocol, any prescribed convergence time can be guaranteed regardless of the initial conditions.
- The Implicit Lyapunov Function (ILF) method for finite-time stability analysis has been introduced in [75]. The control algorithm for finite-time stabilization of a chain of integrators has been developed. The scheme of control parameters selection has been presented by LMIs. The robustness of the finite-time control algorithm with respect to system uncertainties and disturbances has been studied. The new high order sliding mode control has been derived as a particular case of the developed finite-time control algorithm. The settling time estimate has been obtained using ILF method. The algorithm of practical implementation of the ILF control scheme has been discussed.

6.2. Model-free control

The model free control techniques form a new and quickly developing area of control theory. It has been established by the team members and nowadays these tools find many practical applications and attract a lot of attention due to their clear advantages for designers: they provide a control law independently in the model knowledge. The achievements obtained in 2013 are as follows:

- A new development of the model-free control theory with application to active magnetic bearing control have been presented in [53].
- "Model-free control" and the corresponding "intelligent" PID controllers (iPIDs), which already had many successful concrete applications, have been presented in [27] for the first time in a unified manner, where the new advances have been taken into account.
- In [62], it is shown that the "intelligent" controllers, which are associated to the recently introduced model-free control synthesis, may be easily implemented on cheap and small programmable devices.
- An application of the model-free control for regulation of the water level under several constraints has been reported in [40].

6.3. Algebraic technique for estimation, differentiation and its applications

Elementary techniques from operational calculus, differential algebra, and non-commutative algebra lead to a new algebraic approach for estimation and detection. It is investigated in various areas of applied sciences and engineering. The following lists only some applications:

- Design of a stabilizing feedback based on acceleration measurements and an algebraic state estimation method has been proposed in [54].
- An extension of the algebraic differentiation method to fractional derivatives calculation in continuous and discrete time has been studied in [88] and [89] respectively. Applications to identification and parameter estimation of fractional linear systems have been considered in [67], [68].
- Smoothing noisy data with spline functions is well known in approximation theory. Smoothing splines have been already used to deal with the problem of numerical differentiation. In [43], we extend this method to estimate the fractional derivatives of a smooth signal from its discrete noisy data. We begin with finding a smoothing spline by solving the Tikhonov regularization problem. Then, we propose a fractional order differentiator by calculating the fractional derivative of the obtained smoothing spline.
- In [81], we apply an algebraic method to estimate the amplitudes, phases and frequencies of a biased and noisy sum of complex exponential sinusoidal signals. The obtained estimates are integrals of the noisy measured signal: these integrals act as time-varying filters.

6.4. Observability and observer design for nonlinear systems

Observability analysis and observer design are important issues in the field of control theory. Some recent results are listed below:

- An epistemology of observation theory and its application in the design of software sensor in power electronics have been presented in [42].
- New results on observability and detectability of singular linear systems with unknown inputs have been developed in [12].
- The paper [47] supplies a new algorithm to compute the internal dynamics (or inversion dynamics) of affine MIMO control nonlinear systems.
- The design of observers for nonlinear systems with unknown, time-varying, bounded delays, on both state and input, still constitutes an open problem. In [28], we show how to solve it for a class of nonlinear systems by combining the high gain observer approach with a Lyapunov-Krasovskii functional. Sufficient conditions have been provided to prove the practical stability of the observer.

- An influence of restricted isometry property to the observability under sparse measurements has been analyzed in [65].
- The paper [38], [79] concerns the design of a nonlinear observer through a transformation of a nonlinear system into an observer form that supports a high gain observer. Sufficient geometrical condition has been deduced to guarantee the existence of change of coordinates allowing the transformation of a nonlinear system into the proposed normal form. In [80], the Partial Observability Normal Forms (PONF) of nonlinear dynamical systems have been investigated. Necessary and sufficient conditions for the existence of a diffeomorphism bringing the original nonlinear system into a PONF have been established.

6.5. Sliding mode control and estimation

Sliding mode algorithms are very popular for finite-time estimation and regulation. The recent results obtained by the group are as follows:

- Some constructive approximations and an alternative theoretic characterization of some classes of sliding mode control processes has been presented in [11].
- In [64] we investigate observer design under sparse measurement, i.e. under Nyquist-Shannon frequency. An analysis demonstrates that it is impossible to use only a high order sliding mode observer in the case of sparse measurement. Then it has been shown that a high order sliding mode observer coupled with an impulsive observer is a pertinent solution at least for some particular class of systems.
- Anomaly detection has been an active open problem in the networks community for several years. In [35], we aim at detecting such abnormal signals by control theory techniques. Several classes of sliding mode observers have been proposed for a fluid flow model of the TCP/internet protocol network.
- A sliding mode control has been developed for robust stabilization of fractional-order input-delay linear systems in the presence of uncertainties and external disturbances in [78]. First, a fractional-order state predictor has been used to compensate the delay in the input control. Second, a robust sliding mode control has been proposed in order to stabilize the system and to thwart the effect of model uncertainties and external disturbances. The sliding mode controller has been designed by considering a sliding surface defined by fractional order integral.

6.6. Non-linear, Sampled and Time-delay systems

Nonlinearities, sampling, quantization and time-delays cause serious obstructions for control and observer design in many fields of techniques and engineering (e.g. networked and internet systems, distributed systems etc.). The proposed by the team algebraic approach suits well for estimation and regulation in such a type of systems. The recent results are listed below:

- The work [59] aims at decreasing the number of sampling instants in state feedback control for perturbed linear time invariant systems. The approach is based on linear matrix inequalities obtained thanks to Lyapunov-Razumikhin stability conditions and convexification arguments that guarantee the exponential stability for a chosen decay-rate.
- A novel self-triggered control, which aims at decreasing the number of sampling instants for the state feedback control of perturbed linear time invariant systems, has been proposed in [60]. The approach is based on convex embeddings that allow for designing a state-dependent sampling function guaranteeing the system's exponential stability for a desired decay-rate and norm-bounded perturbations. One of the main contributions of the paper [60] is an LMI based algorithm that optimizes the choice of the Lyapunov function so as to enlarge the lower-bound of the sampling function while taking into account both the perturbations and the decay-rate.
- In [63], we consider the issue of stabilizing a class of linear systems using irregular sampled output measurements.

- The paper [73] is dedicated to the stability analysis of nonlinear sampled-data systems, which are affine in the input. Assuming that a stabilizing continuous-time controller exists and it is implemented digitally, we intend to provide sufficient asymptotic/exponential stability conditions for the sampled-data system. This allows to find an estimate of the upper bound on the asynchronous sampling periods. The stability analysis problem is formulated both globally and locally. The main idea of the paper is to address the stability problem in the framework of dissipativity theory. Furthermore, the result is particularized for the class of polynomial input-affine sampled-data systems, where stability may be tested numerically using sum of squares decomposition and semidefinite programming.
- The problem of output control design for linear system with unknown and time-varying input delay, bounded exogenous disturbances and bounded deterministic measurement noises has been considered in [77]. The prediction technique has been combined with Luenberger-like observer design in order to provide the stabilizing output feedback. The scheme of parameters tuning for reduction of measurement noises effect and exogenous disturbances effects has been developed using the Attractive Ellipsoids Method.
- Using the theory of non-commutative rings, the paper [39] studies the delay identification of nonlinear time-delay systems with unknown inputs. A sufficient condition has been given in order to deduce an output delay equation from the studied system. Then necessary and sufficient conditions have been proposed to judge whether the deduced output delay equation can be used to identify the delay, which is involved in this equation.

6.7. Interval control and estimation

In many cases due to parametric and/or signal uncertainties presented in a plant model it is not possible to design a conventional observer, which provides a point-wise estimate of state in a finite time or asymptotically. In this case it is still frequently possible to design interval observers, which generate an estimate on the interval of the admissible values of the state at the current instant of time. The recent new results in this field are listed below:

- The work [49] is devoted to interval observer design for Linear Parameter-Varying (LPV) systems under assumption that the vector of scheduling parameters is not available for measurements. Stability conditions are expressed in terms of matrix inequalities, which can be solved using standard numerical solvers. Robustness and estimation accuracy with respect to model uncertainty is analyzed. Two solutions are proposed for nonnegative systems and for a generic case. The efficiency of the proposed approach is demonstrated through computer simulations.
- Development of interval observers for time invariant [55] and time-varying [21] discrete-time systems has been presented by the members of the team.
- Interval estimation for uncertain systems with time-varying delays has been considered in [22], [56]. A reduced-order interval observer has been designed, stability and robustness conditions have been obtained.
- The paper [24] is devoted to design of interval observers for Linear Time Varying (LTV) systems and a class of nonlinear time-varying systems in the output canonical form. An interval observer design is feasible if it is possible to calculate the observer gains making the estimation error dynamics cooperative and stable. It has been shown in [24] that under some mild conditions the cooperativity of an LTV system can be ensured by a static linear transformation of coordinates.
- The problem of output stabilization of a class of nonlinear systems subject to parametric and signal uncertainties has been studied in [25]. First, an interval observer has been designed estimating the set of admissible values for the state. Next, it has been proposed to design a control algorithm for the interval observer providing convergence of interval variables to zero, that implies a similar convergence of the state for the original nonlinear system. An application of the proposed technique shows that a robust stabilization can be performed for linear time-varying and LPV systems without assumption that the vector of scheduling parameters is available for measurements.

- The paper [26] deals with the problem of joint state and parameter estimation based on a set adaptive observer design. The problem is formulated and solved for an LPV system. The resolution methodology avoids the exponential complexity obstruction usually encountered in the set-membership parameter estimation.
- The output stabilization problem for a linear system with an unknown bounded time-varying input delay has been considered in [34], [76]. The interval observation technique has been applied in order to obtain guaranteed interval estimate of the system state. The procedure of the interval observer synthesis uses lower and upper estimates of the unknown delay and requires to solve a special Silvester's equation. The interval predictor has been introduced in order to design a linear stabilizing feedback. The control design procedure is based on LMIs.
- The paper [37] describes a robust set-membership-based Fault Detection and Isolation (FDI) technique for a particular class of nonlinear systems, the so-called flat systems. The proposed strategy consists in checking if the expected input value belongs to an estimated feasible set computed using the system model and the derivatives of the measured output vector. The output derivatives are computed using a numerical differentiator. The set-membership estimator design for the input vector takes into account the measurement noise thereby making the consistency test robust.
- The objective of the work [82] is to develop some design methods of interval observers for a class of nonlinear continuous-time systems. It has been assumed that the estimated system can be represented as a superposition of the nominal subsystem (belonged to the class of uniformly observable systems) and a Lipschitz nonlinear perturbation vanishing at the origin. Then it has been shown that there exists an interval observer for the system that estimates the set of admissible values for the state consistent with the output measurements.

6.8. Networked robots

The mobile robots constitute an important area of practical development for the team:

- The paper [71] presents a path planning algorithm for autonomous navigation of non-holonomic mobile robots in complex environment. The irregular contour of obstacles is represented by segments. The goal of the robot is to move towards a known target while avoiding obstacles. The velocity constraints, kinematic robot model and non-holonomic constraint are considered in the problem. The optimal path planning problem is formulated as a constrained receding horizon planning problem and the trajectory is obtained by solving an optimal control problem with constraints. Local minima are avoided by choosing intermediate objectives based on the real time environment.
- The paper [69] presents a cooperative path planning approach for the navigation of non-holonomic mobile robots in environment with obstacles. Shared information can be obtained by sharing the local information between robots, thus the trajectories can be more optimized. Visibility graph approach is used to generate a series of intermediate objectives which guarantee the robots to reach the final objective without local minima. Then the reach of intermediate objectives is ensured by the optimal path planning algorithm. The velocity constraints, kinematic constraints and non-holonomic constraints of the mobile robot are considered in the problem.
- The paper [70] presents the real-time identification of different types of non-holonomic mobile robot systems. Since the robot type is a priori unknown, the robot systems are formulated as a switched singular nonlinear system, and the problem becomes the real-time identification of the switching signal, and then the existence of the input-output functions and the distinguishability of the systems are studied.
- An intelligent PID controller (i-PID controller) has been applied to control the non-holonomic mobile robot with measurement disturbance in [72]. Because of the particularity of the non-holonomic systems, this paper proposes to use a switching parameter α in the i-PID controller.

6.9. Applications

As it was mentioned, Non-A is a kind of "method-driven" project, which deals with different aspects of finite-time estimation and control. Thus different applications are possible, ones touched this year are as follows (skipping the networked robots considered in the previous section):

- A sensorless speed control for a DC series motor has been presented in [41] based on sliding-mode control and estimation algorithms.
- The paper [48] presents a feasibility study, which aims to demonstrate the applicability of the CNC automation philosophy for the process of AFM probe-based nano machining conducted on commercial AFM instruments.
- An oscillatory failure case detection for aircrafts using non-homogeneous sliding-mode differentiator in noisy environment has been considered in [50].
- Sensorless fault tolerant control for induction motors has been developed in [18].
- The problem of an actuator fault detection in aircraft systems has been considered in [19]. A particular attention has been paid to the oscillatory failure case study.
- In [58], we consider a vehicle equipped with active front steer and rear torque vectoring. While the former adds an incremental steer angle to the driver's input, the latter imposes a torque by means of the rear axle. The active front steer control is actuated through the front tires, while the rear torque vectoring can be actuated through the rear tires. A nonlinear controller using the super-twisting algorithm has been designed in order to track in a finite time the lateral and yaw angular velocity references.
- Systematic and multifactor risk models have been revisited via algebraic methods, which were already successfully developed in signal processing and in automatic control, in [61].
- In [84], we address the problem of approximating scattered data points by C1-smooth polynomial spline curves and surfaces using L1-norm optimization. The use of this norm helped us to preserve the shape of the data even near to abrupt changes.
- As capacitor voltages are necessary for the three-cell DC-DC chopper control, the estimation of such voltages by an observer is attractive solution in terms of cost. However, due to the hybrid behaviour of this structure, the capacitor voltages may be partially or even not observable for a given switching configuration. In other words, the observability matrix associated to the capacitor voltages never has a full rank. In order to make the observer conceivable, the paper [29] proposes a new design by establishing sufficient conditions under which the capacitor voltages can be reconstructed within appropriate specific switching sequence and not necessarily instantly.
- The problem of converters coordination of a fuel cell system involving a hydrogen fuel cell with supercapacitors for applications with high instantaneous dynamic power has been addressed in [32]. The problem is solved by using a non-linear controller based on passivity.
- The paper [66] is devoted to development of control algorithms for nonlinear parametrically uncertain systems. Original system dynamics is approximated by a set of local NARX models combined by a special mixing rule. Algorithm for local models' parameters estimation and structure adjustment has been developed. The developed technique has been applied to the problem of regulation of spark ignition engines.
- The paper [36] is dedicated to the problem of pneumatic cylinder control without pressure measurement. Based on the theory of homogeneous, finite time stable, ordinary differential equations, a state feedback nonlinear controller has been proposed. The closed loop system stability has been proven and an attraction domain of the controller has been given.

CLASSIC Project-Team

5. New Results

5.1. Contributions earlier to 2013 but only published in 2013

Participants: Gérard Biau, Pierre Gaillard, Gilles Stoltz.

We do not discuss here the contributions provided by [14], [12], [13], [16] since they were achieved in 2012 or earlier (but only published this year due to the reviewing and publishing process).

5.2. Approachability with partial monitoring

Participant: Gilles Stoltz.

This line of research has been developed in our team since its creation (see, in particular, the founding article [9] as well as several other publications in the previous reports). Following the earlier contribution on exhibiting an efficient algorithm for approachability with partial monitoring based on some necessary and sufficient dual condition, we study in [15] the primal approach: the statement of the condition and the existence of (efficient or inefficient) algorithms based on it.

5.3. High-dimensional learning and complex data

Participant: Gérard Biau.

We describe four (not so related) contributions on the theme of high-dimensional learning and complex data.
In [17] we address the problem of supervised classification of Cox process trajectories, whose random intensity is driven by some exogenous random covariable. The classification task is achieved through a regularized convex empirical risk minimization procedure, and a nonasymptotic oracle inequality is derived. The results are obtained by taking advantage of martingale and stochastic calculus arguments, which are natural in this context and fully exploit the functional nature of the problem.
The cellular tree classifier model addresses a fundamental problem in the design of classifiers for a parallel or distributed computing world: Given a data set, is it sufficient to apply a majority rule for classification, or shall one split the data into two or more parts and send each part to a potentially different computer (or cell) for further processing? At first sight, it seems impossible to define with this paradigm a consistent classifier as no cell knows the "original data size", n. However, we show in [18] that this is not so by exhibiting two different consistent classifiers.
A new method for combining several initial estimators of the regression function is introduced. Instead of building a linear or convex optimized combination over a collection of basic estimators $r_1, \cdots, r_M$, [19] uses them as a collective indicator of the proximity between the training data and a test observation. This local distance approach is model-free and very fast. More specifically, the resulting collective estimator is shown to perform asymptotically at least as well in the L^2 sense as the best basic estimator in the collective. A companion R package called COBRA (standing for COmBined Regression Alternative) is presented (downloadable on http://cran.r-project.org/web/packages/COBRA/index.html). Substantial numerical evidence is provided on both synthetic and real data sets to assess the excellent performance and velocity of the method in a large variety of prediction problems.
The impact of letting the dimension d go to infinity on the L^p-norm of a random vector with i.i.d. components has surprising consequences, which may dramatically affect high-dimensional data processing. This effect is usually referred to as the *distance concentration phenomenon* in the computational learning literature. Despite a growing interest in this important question, previous work has essentially characterized the problem in terms of numerical experiments and incomplete mathematical statements. In the paper [20], we solidify some of the arguments which previously appeared in the literature and offer new insights into the phenomenon.

5.4. Dimension free principal component analysis

Participants: Olivier Catoni, Ilaria Giulini.

In a work in progress, Ilaria Giulini, as part of her PhD studies, proved the following dimension free inequality, related to Principal Component Analysis in high dimension. Given an i.i.d. sample X_i, $1 \leq i \leq n$ of vector valued random variables $X_i \in \mathbf{R}^d$, there exists an estimator $\widehat{N}$ of the quadratic form $N(\theta) = \mathbf{E}(\langle \theta, X \rangle^2)$ such that for any $n \leq 10^{20}$, with probability at least $1 - 2\epsilon$, for any $\theta \in \mathbf{R}^d$,

$$\mathbf{1}\left(4\mu < 1\right) \left| \frac{\widehat{N}(\theta)}{N(\theta)} - 1 \right| \leq \frac{\mu}{1 - 4\mu},$$

where

$$\mu = \sqrt{\frac{2.07\ (\kappa - 1)}{n} \left[\log\left(\epsilon^{-1}\right) + 4.3 + \frac{1.6\ \|\theta\|^2 \mathbf{Tr}(G)}{N(\theta)} \right]} + \sqrt{\frac{184\ \kappa \|\theta\|^2 \mathbf{Tr}(G)}{nN(\theta)}},$$

where $G = \mathbf{E}\left(XX^\top\right)$ is the Gram matrix and where $\kappa = \sup \left\{ \dfrac{\mathbf{E}\left(\langle \theta, X \rangle^4\right)}{\mathbf{E}\left(\langle \theta, X \rangle^2\right)^2}, \theta \in \mathbf{R}^d \smallsetminus \mathbf{Ker}(G) \right\}$ is some kurtosis coefficient. This result proves that the expected energy in direction θ can be estimated at a rate that is independent of the dimension of the ambient space $\mathbf{R}^d$. It is obtained using PAC-Bayes inequalities with Gaussian parameter perturbations. The same bound holds in a Hilbert space of infinite dimension, opening the possibility of a rigorous mathematical study of kernel principal component analysis of random data, where the data are represented in a possibly infinite dimensional reproducing kernel Hilbert space.

5.5. Statistical models for corpus linguistics

Participants: Olivier Catoni, Thomas Mainguy.

In [21] we describe a language model as the invariant measure of a Markov chain on sentence samples. The kernel of this Markov chain is defined with the help of some context free grammars : from the sentence sample, a random parse model produces a context free grammar with weighted rules, and from this grammar, a new sentence sample is formed by applying the rules randomly. We prove various mathematical properties of this Markov process, related to its computation cost and the fact that it is weakly reversible and therefore ergodic on each of its communicating classes. As a companion to the Markov chain on sentence samples, we can also define a Markov chain on weighted context free grammars. This leads to another type of grammar, that we called Toric Grammars, defined by a family of context tree grammars that can be computed from any of its members as the communicating class of a Markov chain on context free grammars with weighted rules. Preliminary simulations on small data sets are very encouraging, in that they show that this type of model is able to grasp the recursive nature of natural languages.

DOLPHIN Project-Team

6. New Results

6.1. Bi-level multi-objective optimization for pricing problems in long-haul transportation

Participants: M. Diaby, L. Brotcorne and E-G. Talbi

This work is concerned with the problem of pricing for a long-haul full load goods transportation. More precisely, we are interested in the situation where each vehicle delivers single request at a time. In this environment, we study the problem of pricing and valorization of unutilized capacity between two carriers. The first carrier B, cannot serve all the transportation requests and he thus needs to use outsourcing : second carrier A or his competitors. Carrier A, has to define the prices for carrier B transportation requests. Once carrier A has given its prices for the operations, it is B's decision to turn to A or to another carrier. This sequential and non-cooperative decision-making process can be adequately represented as a bilevel program : carrier B (the follower) wants to minimize transportation cost while A (the leader) seeks to maximize the revenue. Carrier A explicitly incorporates the reaction of carrier B in his optimization process.

Two types of models have been proposed : the bilevel mono-objective model and the bilevel biobjective model. More precisely, two objectives are simultaneously considered for the leader problem : the maximization of revenue and balancing the free load length (limiting the free load distances). We propose exact methods to solve moderate size instance of the problem and the heuristics to solve large-scale instances in reasonable time.

6.2. Approximating multi-objective scheduling problems

Participant: El-ghazali Talbi
External participants: Said Dabia, Tom Van Woensel, Tom De Kok (Eindhoven Technical University)

In this contribution, we propose a generic approach to deal with multi-objective scheduling problems (MOSPs). The aim is to determine the set of Pareto solutions that represent the interactions between the different objectives. Due to the complexity of MOSPs, an efficient approximation based on dynamic programming is developed. The approximation has a provable worst case performance guarantee. Eventhough the approximate Pareto set consists of fewer solutions, it represents a good coverage of the true set of Pareto solutions. We consider generic cost parameters that depend on the state of the system. Numerical results are presented for the time-dependent multi-objective knapsack problem, showing the value of the approximation in the special case when the state of the system is expressed in terms of time [23].

6.3. Force-Based Cooperative Search Directions in Evolutionary Multi-objective Optimization

Participants: Bilel Derbel, Dimo Brockhoff, Arnaud Liefooghe

In order to approximate the set of Pareto optimal solutions, several evolutionary multi-objective optimization (EMO) algorithms transfer the multi-objective problem into several independent single-objective ones by means of scalarizing functions. The choice of the scalarizing functions' underlying search directions, however, is typically problem-dependent and therefore difficult if no information about the problem characteristics are known before the search process. In [46], we present new ideas of how these search directions can be computed *adaptively* during the search process in a *cooperative* manner. Based on the idea of Newton's law of universal gravitation, solutions attract and repel each other *in the objective space*. Several force-based EMO algorithms are proposed and compared experimentally on general bi-objective ρMNK landscapes with different objective correlations. It turns out that the new approach is easy to implement, fast, and competitive with respect to a $(\mu + \lambda)$-SMS-EMOA variant, in particular if the objectives show strong positive or negative correlations.

6.4. DYNAMO (DYNAmic programming using Metaheuristic for Optimization Problems)

Participants: Sophie Jacquin, Laetitia Jourdan, El-Ghazali Talbi

DYNAMOP (DYNAmic programming using Metaheuristic for Optimization Problems) is a new dynamic programming based on genetic algorithm to solve a hydro-scheduling problem. The representation which is based on a path in the graph of states of dynamic programming is adapted to dynamic structure of the problem and it allows to hybridize easily evolutionary algorithms with dynamic programming. DYNAMOP has been tested on two case studies of hydro-scheduling problem with different price scenarios. Experiments indicate that the proposed approach performs considerably better than classical genetic algorithms and dynamic programming.

6.5. MOCA-I: Multi-Objective Classification Algorithm for Imbalanced Data

Participants: Julie Jacques, Clarisse Dhaenens, Laetitia Jourdan

Dealing with Imbalanced data is a real challenge as predicting the minority class may be very difficult but has a great interest for medical applications for example. Therefore, we propose MOCA-I, a new multi-objective local search algorithm that is conceived to deal with class imbalancy, double meaning of missing data, volumetry and need of highly interpretable results all together [50]. MOCAI is a Pittsburgh multi-objective partial classification rule mining algorithm, using dominance-based multi-objective local search (DMLS). In comparison to state-of-the-art classification algorithms, MOCA-I obtains the best results on the 10 data sets of literature and is statistically better on the real data sets [50].

6.6. Neutrality Analysis is Graph coloring problem

Participants: Aymeric Blot, Clarisse Dhaenens, Laetitia Jourdan, Marie-Eleonore Marmion

Solving neutral problems is challenging as many optimization methods have difficulty to obtain good solutions. Hence, studying the neutrality in order to provide insights on the structure of the problem to be soved may be an answer. This has been done for the graph coloring problem (GCP) for which the neutrality of some hard instances has been quantified. This neutrality property has to be detected as it impacts the search process. Indeed, local optima may belong to plateaus that represent a barrier for local search methods. Then, we also aim at pointing out the interest of exploiting neutrality during the search. Therefore, a generic local search dedicated to neutral problems, NILS, is performed on several hard instances [78].

6.7. Neutrality in Multi-objective Local Search

Participants: Aymeric Blot, Clarisse Dhaenens, Laetitia Jourdan
External Participants: Hernan Aguirre, Kiyoshi Tanaka - Shinshu University, Japan

In multi-objective combinatorial optimization, the dominance-based local search algorithms are faced to sets of non-comparable solutions. In the absence of preferences, these solutions are equally good from the Pareto dominance perspective and can be considered neutral in term of quality, similar to the solutions who shares the same fitness value in mono-objective optimization. We propose two ideas to use the neutrality to improve the current local search algorithms. First, we analyze the distribution of neighbors for both small fully enumerable instances and hard large instances, to understand the distribution of neutral neighbors according to the rank of the solutions. Then, we compare the results of the proposed algorithms with the standard ones according to different indicators.

6.8. Biclustering for GWA data

Participants: Khedidja Seridi, Laetitia Jourdan, El-Ghazali Talbi

We have examined the possibilities of applying biclustering approaches to detect association between SNP markers and phenotype traits. There- fore, we have proposed a multiobjective model for biclustering problems in GWA context. Furthermore, we have proposed an adapted heuristic and meta- heuristic to solve it. The good performances of our algorithms are assessed using synthetic data sets.

6.9. Fitness Landscape Analysis for Multiobjective Optimization

Participant: Arnaud Liefooghe
External participants: Hernan Aguirre, Kiyoshi Tanaka (Shinshu Univ., Japan), Sébastien Verel (Univ. Littoral Côte d'Opale, France)

In [57], we investigate the correlation between the characteristics extracted from the problem instance and the performance of a simple evolutionary multiobjective optimization algorithm. First, a number of features are identified and measured on a large set of enumerable multiobjective NK-landscapes with objective correlation. A correlation analysis is conducted between those attributes, including low-level features extracted from the problem input data as well as high-level features extracted from the Pareto set, the Pareto graph and the fitness landscape. Second, we experimentally analyze the (estimated) running time of the global SEMO algorithm to identify a $(1+\epsilon)$-approximation of the Pareto set. By putting this performance measure in relation with problem instance features, we are able to explain the difficulties encountered by the algorithm with respect to the main instance characteristics.

In [38], we study the effects of population size on selection and performance scalability of two dominance-based algorithms applied to many-objective optimization. Our aim is to understand the relationship between the size of the Pareto optimal set, a characteristic of the many-objective problem at hand, the population size and the ability of the algorithm to retain Pareto optimal solutions in its population and find new ones. This work clarifies important issues of the dynamics of evolutionary algorithms on many-objective landscapes, particularly related to survival selection. It shows that optimal solutions are dropped from the population in favor of suboptimal solutions that appear non-dominated when survival selection is applied. It also shows that this selection lapse, the dropping of optimal solution, affects the discovery of new optimal solutions and is correlated to population size and the distribution of solutions that survival selection renders. Selection makes less mistakes with larger populations and when the distribution of solutions is better controlled. The results of this study will be helpful to properly set population size and have a clearer idea about the performance expectation of the algorithm.

6.10. On Set-based Local Search for Multiobjective Combinatorial Optimization

Participant from DOLPHIN: Arnaud Liefooghe
External participants: Matthieu Basseur, Adrien Goëffon (Univ. Angers, France), Sébastien Verel (Univ. Littoral Côte d'Opale, France)

In [42], we formalize a multiobjective local search paradigm by combining set-based multiobjective optimization and neighborhood-based search principles. Approximating the Pareto set of a multiobjective optimization problem has been recently defined as a set problem, in which the search space is made of all feasible solution-sets. We here introduce a general set-based local search algorithm, explicitly based on a set-domain search space, evaluation function, and neighborhood relation. Different classes of set-domain neighborhood structures are proposed, each one leading to a different set-based local search variant. The corresponding methodology generalizes and unifies a large number of existing approaches for multiobjective optimization. Preliminary experiments on multiobjective NK-landscapes with objective correlation validates the ability of the set-based local search principles. Moreover, our investigations shed the light to further research on the efficient exploration of large-size set-domain neighborhood structures.

6.11. Feature selection in high dimensional regression problems for genomics

Participants: Julie Hamon, Clarisse Dhaenens (External collaborator : Julien Jacques)

In the context of genomic selection in animal breeding, an important objective consists in looking for explicative markers for a phe-notype under study. In order to deal with a high number of markers, we propose to use combinatorial optimization to perform variable selection. Results show that our approach outperforms some classical and widely used methods on simulated and "closed to real" datasets [76]. Familial relationships have also been used in this specific context and allow to improve results.

6.12. Indicator-Based Multiobjective Optimization

Participant: Dimo Brockhoff
External Participants: Johannes Bader (formerly at ETH Zurich, Switzerland), Youssef Hamadi (Microsoft Research, Cambridge, UK), Souhila Kaci (Université Montpellier 2, France), Lothar Thiele (ETH Zurich, Switzerland), Heike Trautmann (University of Munster, Germany) Tobias Wagner (TU Dortmund, Germany), and Eckart Zitzler (PH Bern, Switzerland)

Indicator-based (evolutionary) multiobjective optimization algorithms have been first introduced in 2004 and typically use a quality indicator, assigning a solution set a real value, as a direct, internal performance criterion. Given that the indicator and the number μ of desired points is fixed, the optimization goal, also denoted by the term *optimal μ-distribution*, is then defined as the solution set(s) of size μ which maximizes the indicator value.

In 2013, we continued to investigate, theoretically and numerically, the optimal μ-distributions for the R2 indicator, an often recommended indicator based on scalarization functions [73]. We also proposed a new multiobjective optimizer with an R2-indicator-based selection [70]. With respect to the even more common *hypervolume indicator*, we combined the idea of the weighted hypervolume indicator with the idea of interactive algorithms and proposed a new algorithm that adapts the weighted hypervolume's weight function according to the user's preferences during the search. Last, we summarized our knowledge on the weighted hypervolume indicator and proposed a general framework of how to employ it within the hypervolume-based W-HypE algorithm [18].

6.13. A Hybrid Metaheuristic for Multiobjective Unconstrained Binary Quadratic Programming

Participant : Arnaud Liefooghe
External participants : Jin-Kao Hao (Univ. Angers, France), Sébastien Verel (Univ. Littoral Côte d'Opale, France)

The conventional Unconstrained Binary Quadratic Programming (UBQP) problem is known to be a unified modeling and solution framework for many combinatorial optimization problems. In [29], we extend the single-objective UBQP to the multiobjective case (mUBQP) where multiple objectives are to be optimized simultaneously. We propose a hybrid metaheuristic which combines an elitist evolutionary multiobjective optimization algorithm and a state-of-the-art single-objective tabu search procedure by using an achievement scalarizing function. Finally, we define a formal model to generate mUBQP instances and validate the performance of the proposed approach in obtaining competitive results on large-size mUBQP instances with two and three objectives.

6.14. Multi-core GPU-based parallel optimization

We have mainly investigated the design and implementation on multi-core GPU-based platforms of meta-heuristics and tree-based exact optimization methods focusing on Branch and bound (B&B) algorithms (Ph.D thesis of I. Chakroun).

- **GPU-based Metaheuristics**
  Participants: N. Melab, T-V. Luong, K. Boufaras and N. Melab

We came out with a pioneering work on single-solution methods. The hierarchy of parallel models has been rethought on GPU dealing with CPU-GPU data transfer optimization, thread control and automatic mapping of candidate solutions to threads. The implementation of the proposed approaches is provided through ParadisEO-GPU in [62] (nominated for Best Paper Award). High speedups ups have been achieved for some problems.

- **Multi-core GPU-based B&B algorithms**
  For exact optimization, we have revisited the design and implementation of highly irregular B&B algorithms on GPU dealing with hierarchical device memory optimization, on GPU combined with multi-core [45] dealing with CPU-GPU data transfer optimization and work partitioning, and on GPU-enhanced computational grids. Accelerations up to $\times 217$ are achieved on Tesla Nvidia C2050 on large Flow-Shop problems.

6.15. Energy-aware scheduling for clouds

Participants: Y. Kessaci, N. Melab, E-G. Talbi

High-performance computing (HPC) is moving from in-house to cloud-based HPC. One of the major issues of this later is the scheduling of HPC applications taking into account the energy criterion in addition to performance. In [54], we have addressed that issue (Ph.D thesis of Y. Kessaci). We have proposed several metaheuristics for cloud managers and experimented on OpenNebula using different (VMs) arrival scenarii and different hardware infrastructures. The results show that our approaches outperform the scheduler provided in OpenNebula by a significant margin in terms of energy consumption and number of scheduled VMs.

6.16. Heterogenous Multi-CPU Multi-GPU Parallel Branch-and-Bound Tree Search

Participants: Trong-Tuan Vu, Bilel Derbel, Nouredine Melab
In this work [71], we push forward the design of parallel and distributed optimization algorithms running on heterogenous systems consisting of multiple CPUs coupled with multiple GPUs. We consider parallel Branch-and-Bound (B&B), viewed as a generic algorithm searching in a dynamic tree representing a set of candidate solutions built dynamically at runtime. Given that several distributed CPUs and GPUs coming from possibly different clusters connected through a network can be used to parallelize the tree search, we give new insights into how to fully benefit from such a heterogeneous environment. More precisely, we describe a two-level generic and fully distributed parallel approach taking into account PU characteristics. In the first level, we use data streaming in order to allow parallelism between hosts and devices. The evaluation of tree nodes is done inside a GPU while the CPU-host is performing the pruning, selection and decomposition operations in parallel. In the second level, our approach incorporates an adaptive dynamic load balancing scheme based on distributed work stealing, in order to flow workloads efficiently from overloaded PUs to idle ones at runtime. We deployed our approach over a distributed system of up to 20 GPUs and 128 CPUs coming from three clusters. Different scales and configurations of PUs were experimented with the B&B algorithm and the well-known FlowShop combinatorial optimization problem as a case study. Firstly, on one single GPU, we improve on the running time of previous B&B GPUs implementation by at least a factor of two. More importantly, independently of CPUs or GPUs scale or power, our approach provides a substantial speed-up which is *nearly optimal* compared to the ideal performance one could expect in theory.

GEOSTAT Project-Team

6. New Results

6.1. Nonlinear dynamics and Mild Therapeutic Hypothermia (MTH)

Participants: Binbin Xu [correspondant], Oriol Pont, Hussein Yahia, Ihu Liryc.

The neurological damage after cardiac arrest constitutes a big challenge of hospital discharge. The mild therapeutic hypothermia (MTH) (34°C - 32°C) has shown its benefit to reduce this type of damage. However, it can have many adverse effects, among which the cardiac-arrhythmia-generation-a-posteriori (CAGP) can represent up to 34%. So it's important to understand the mechanism of CAGP in order to improve this therapy. Our study with a cardiac culture in vitro showed that at 35°C the CAGP can be induced. Spiral waves, commonly considered as a sign of cardiac arrhythmia, are observed. The process of MTH can be represented by a Pitchfork bifurcation, which could explain the different ratio of arrhythmia among the adverse effects after this therapy. This nonlinear dynamics suggests that a variable speed of cooling / rewarming, especially when passing 35°C, would help to decrease the ratio of post-hypothermia arrhythmia and then improve the hospital output. See figures 5 , 6 .

Figure 5. Phase space reconstruction for extracellular potential signals at 37°C, 35°C and 33°C.

Publications: [33], [35], [39].

6.2. Characterizing cardiac arrhythmias and their mechanisms by means of nonlinear and robust methods

Participants: Oriol Pont [correspondant], Binbin Xu, Hussein Yahia, Ihu Liryc.

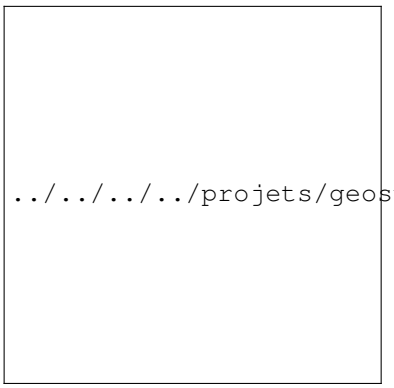


Figure 6. Illustration of Bifurcation or Trifurcation (type Pitchfork) of hypothermia effect.

Nonlinear analysis provides appropriate tools to characterize cardiac dynamics. Singularity analysis and phase-space reconstruction are physically meaningful complexity measures with minimal assumptions on the underlying models. These methods are based on effective descriptions derived from first principles, and as a consequence, parameters are robustly estimated. We have validated this approach on ECG, endocavitary catheter measures and electrocardiographic maps.

Key parameters vary infrequently and exhibit sharp transitions, which show where information concentrates and correspond to actual dynamical regime changes. Singularity exponents sift a simple fast dynamics from its slow modulation. In space domain, extreme values highlight arrhythmogenic areas. We observe a correspondence of time lag fluctuations of phase-space reconstructions with atrial fibrillation episodes in the same way as with the dynamical changes coming from singularity exponents. This characterization of information transitions could be used in the regularization of inverse-problem mapping of electrocardiographic epicardial maps. Furthermore, this opens the way for improved model-independent complexity descriptors to be used in non-invasive, automatic diagnosis support and ablation guide for electrical insulation therapy, in cases of arrhythmias such as atrial flutter and fibrillation.
Publications: [34], [29], [32], [37], [21].

6.3. Multifractal Deep Convolutional Pooling for Robust Texture Discrimination

Participants: Hicham Badri [correspondant], Hussein Yahia, Khalid Daoudi.

A robust and fast affine invariant texture classification system is presented. The new approach consists first in filtering the input image with multiple wavelet filters of different scales and orientations followed by a dual-pooling operation to increase the local invariance. The process is repeated for different wavelet sets and multiple image resolutions. This can be seen as a deep convolutional network where the outputs correspond to the pooling responses. The next step consists in extracting a robust affine invariant descriptor based on the scale invariance prior observed in natural images ; a multifractal log exponent histogram is calculated for each output node of the network. These log- histograms are combined to form the main descriptor. The final step consists in features post-processing based on the sparse wavelet coefficients prior to reduce the influence of small perturbations. For the training, we propose a combination of the generative PCA classifier with multiclass SVMs which improves classification rates. We also propose to use multi-illumination and multi-scale training ; two simple strategies to significantly boost classification results when dealing with small and homogeneous training sets. Experiments demonstrate that the proposed solution outperforms existing methods on three challenging public benchmark datasets.

Work submitted to CVPR 2014.

6.4. Nonlinear reconstruction of optical phase perturbated by atmospheric turbulence in Adaptive Optics

Participants: Suman Maji [correspondant], Hussein Yahia, Thierry Fusco.

A new approach to wavefront phase reconstruction in Adaptive Optics (AO) from the low-resolution gradient measurements provided by a wavefront sensor, using a nonlinear approach derived from the Microcanonical Multiscale Formalism (MMF). MMF comes from established concepts in statistical physics, it is naturally suited to the study of multiscale properties of complex natural signals, mainly due to the precise numerical estimate of geometrically localized critical exponents, called the singularity exponents. These exponents quantify the degree of predictability, locally, at each point of the signal domain, and they provide information on the dynamics of the associated system. We show that multiresolution analysis carried out on the singularity exponents of a high-resolution turbulent phase (obtained by model or from data) allows a propagation along the scales of the gradients in low-resolution (obtained from the wavefront sensor), to a higher resolution. We compare our results with those obtained by linear ap- proaches, which allows us to offer an innovative approach to wavefront phase reconstruction in Adaptive Optics.
Supporting grant: Conseil Régional Aquitaine project and funding *OPTAD*.
PhD thesis defended: Suman Kumar Maji, *Multiscale Methods in Signal Processing for Adaptive Optics* , University Bordeaux-1, PhD defended on November 14th, 2013, supervisor: H. Yahia [14].
Publications: [19], [20], [28], [14].

6.5. Nonlinear Speech Analysis

Participants: Vahid Khanagha [correspondant], Khalid Daoudi, Safa Mrad, Nicolas Vinuesa, Blaise Bertrac.

1. *MMF for speech analysis* : we continued our research on the adaptation and application of the MMF to speech analysis and started a research theme on pathological voice analysis. We proposed a novel a compact representation of speech which consists in reconstructing a speech signal form its most singular manifold. This leads us to build a speech waveform coder which outperforms the G.726 standard. We then used our recently developed algorithm for Glottal Closure Instants (GCI) detection to improve the performance of our sparse linear prediction method. We also used this algorithm to develop new acoustic perturbation measures for normal/pathological voice classification.
2. *Matching pursuit for speech analysis* : we first showed that the Gabor dictionary is actually more efficient than the Gammatone dictionary for speech coding using the matching pursuit (MP) algorithm. This results mitigates some famous findings on the neural coding at the human auditory nerve. Second, we shoed that one single parameter, derived from MP decomposition of speech, allow discrimination between normal and dysphonic voices with an accuracy which is significantly higher than all existing methods.

Supporting grant: Inria CORDIS.
PhD thesis defended: Vahid Khanagha *Novel Multiscale Methods for Nonlinear Speech Analysis* , University Bordeaux-1, PhD defended on January 16th, 2013, supervisors: K. Daoudi and H. Yahia [13].
Publications: [17], [27], [41], [40], [44].

6.6. Discriminative learning for Automatic speaker recognition

Participants: Khalid Daoudi [correspondant], Reda Jourani, Régine André Obrecht, Driss Aboutajdine.

We proposed a speaker identification which combines SVM and Large Margin Gaussian Mixture Models (LM-GMM) which outperforms the performance of our LM-GMM system.
Publication: [26].

6.7. Learning Multifractal Structures in Images

Participants: Hicham Badri [correspondant], Hussein Yahia, Driss Aboutajdine.

Learning dictionaries has become a powerful tool in many image processing applications. However, standard learning methods such as K-SVD and Online learning do not take into account the the structure of the patches : each patch is expressed as a linear combination of atoms of one global dictionary. We present a new dictionary learning method which takes into account the nature of each patch by performing a multifractal decomposition of the image. As a result, each fractal set will have a specific dictionary and each dictionary contains atoms of a certain singularity degree. Each patch can therefore be expressed much more efficiently compared to global dictionary learning methods. Current experiments in image denoising show that the proposed method outperforms the global dictionary learning methods.
Work in progress.

6.8. Super resolution maps of partial pressure pCO_2 between the ocean and the atmosphere

Participants: Hussein Yahia [correspondant], Véronique Garçon (laboratoire d'Etudes En Géophysique Et Océanographie Spatiales (legos)), Joël Sudre (laboratoire d'Etudes En Géophysique Et Océanographie Spatiales (legos)), Christoph Garbe (university Of Heidelberg), Christophe Maes (laboratoire d'Etudes En Géophysique Et Océanographie Spatiales (legos)), André Butz (karlsruhe Institute Of Technology (kit)), Boris Dewitte (laboratoire d'Etudes En Géophysique Et Océanographie Spatiales (legos)), Isabelle Dadou (université Paul Sabatier).

Multiresolution analysis computed on singularity exponents estimated from physical variables is used to produce submesoscale (pixel size: 4 kms) of partial pressures pCO_2 maps between the ocean and the atmosphere. Low resolution pCO_2 information coming from models and data is propagated across the scale of the specific multriresolution analysis to infer super resolution pCO_2 maps. Validation with model outputs and boat campaigns.
Supporting grant: OceanFlux project.
Publications: [30], [38].

6.9. Turbulent ocean dynamics at super resolution: validation

Participants: Hussein Yahia [correspondant], Véronique Garçon, Joël Sudre.

Synoptic determination of ocean circulation using data acquired from space, with a coherent depiction of its turbulent characteristics, from large scale ocean circulation down to super resolution of remote sensing optical sensors, remains a fundamental challenge in Oceanography. This determination has the potential of revealing all aspects of the ocean's dynamic variability on a wide range of spatio-temporal scales and will enhance our understanding of ocean-atmosphere exchanges at super resolution, as required in the present context of climate change. We show a 4-year time series of spatial super resolution (4 kms) turbulent ocean dynamics generated from satellite data using emerging nonlinear physics, low resolution dynamics and super resolution oceanic sea surface temperature data. The method at its core consists in propagating across the scales the low resolution dynamics in a multi resolution analysis computed on adimensional critical transition information. The resulting vector field is validated with Lagrangian buoy data at super resolution obtained from NASA Global Drifter Program.
A movie showing the evolution of turbulent ocean dynamics around South Africa in the Algunas current has been made with the help and support of Inria DIRCOM project (C. Blonz, P.-O. Gaumin).
Supporting grant: ICARODE project.
Publications: [30], [38].

6.10. Upwelling

Participants: Ayoub Tamim [correspondant], Khalid Daoudi, Hussein Yahia, Joël Sudre.

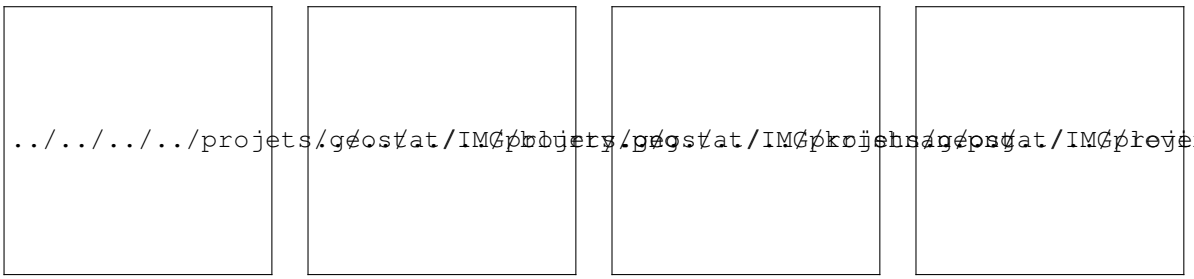
Based on fuzzy clustering, we developed a new algorithm for the segmentation of upwelling regions in the southern atlantic Morrocan coast using Sea Surface temperature images. This method has the advantage of being more efficient and more accurate than a state-of-the-art method. It is followed by a work under way of determinig oriented contours using the MMF.

Publication: [31].

6.11. Combining Local and Non-Local Priors For Image Deconvolution

Participants: Hicham Badri [correspondant], Hussein Yahia.

Non-blind deconvolution consists in recovering a sharp latent image from a blurred image with a known kernel. Deconvolved images usually contain unpleasant artifacts due to the ill-posedness of the problem even when the kernel is known. Making use of natural sparse priors has shown to reduce ringing artifacts but handling noise remains limited. On the other hand, non-local priors have shown to give the best results in image denoising. We propose in this project to combine both local and non-local priors in one framework. By studying the distribution of the singularity exponents as well as the distribution of the eigenvalues of similar patches, we show that the blur increases the self-similarity within an image and thus makes the non-local prior a good choice for denoising blurred images. The blurred image is denoised using only the self-similarties within the image, without any prior specific to the blur, via low rank estimation. However, denoising introduces outliers which are not Gaussian and should be well modeled. Experiments show that our method produces a much better image reconstruction both visually and empirically compared to some popular methods. See figure 7 . Work in progress.



(a) Blurred and Noisy, $\sigma = 2\%$ (b) Krishnan (NIPS 2009) (c) Levin (SIGGRAPH 2007) (d) Proposed

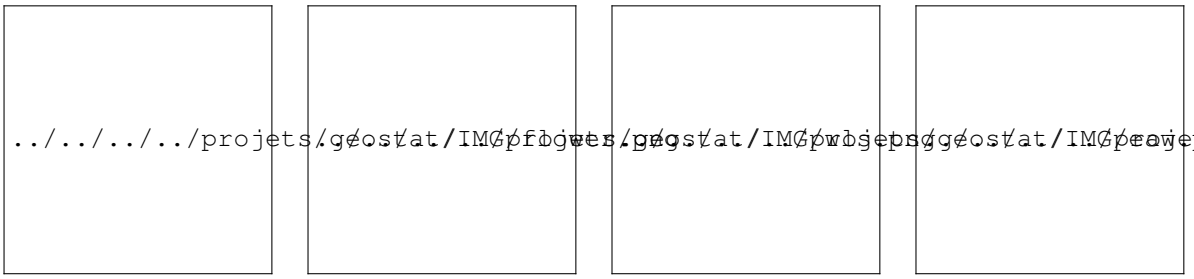
Figure 7. Various deconvolution results. The proposed method produces a much better reconstruction ; note the background noise in the methods (b) and (c). The PSNR is higher with our method 29.56 dB compared to the methods (b) 27.22 dB and (c) 28.11 dB.

6.12. Fast Multi-Scale Detail Decomposition via Accelerated Iterative Shrinkage

Participants: Hicham Badri [correspondant], Hussein Yahia, Driss Aboutajdine.

Edge-aware smoothing is one of the most important operations in computer graphics and vision. It is the building-block for a wide range of applications including : smoothing, detail manipulation, HDR tone-mapping, to cite a few. However, good quality edge-aware smoothing operators are relatively slow. We present a fast solution for performing high-quality edge-aware smoothing, particularly efficient for edge manipulation applications. Our strategy to perform smoothing consists in using a half-quadratic solver with a non-convex sparsity-inducing norm, accelerated using a first order approximation. First, we show how to solve optimization problems with complex non-convex norms using a first order proximal estimation. This step is of

paramount importance not just for smoothing, but for many applications requiring the use non-convex norms. Secondly, we design two norms inspired by natural image statistics. We incorporate these norms with a first order proximal estimation to design the main smoothing operator. Finally, we propose a warm-start solution to accelerate the solver. Experiments show that our method produces high quality results, sometimes better than some state-of-the-art methods, with reduced processing time. We demonstrate the performance of the proposed approach on various applications such as smoothing, multi-scale detail manipulation of low and high dynamic range images as well as high definition video manipulation. See figure 8 .
Work presented at SIGGRAPH Asia 2013 (technical brief), Hong Kong [24].



(a) (b) (c) (d)

Figure 8.

Detail manipulation example. The proposed method produces a high-quality result with reduced processing time. From left to right:(a) Input, (b) WLS, (c) EAW, (d) Proposed method.

6.13. Robust Surface Reconstruction via Triple Sparsity

Participants: Hicham Badri [correspondant], Hussein Yahia, Driss Aboutajdine.

Reconstructing a surface/image from corrupted gradient fields is a crucial step in many imaging applications where a gradient field is subject to both noise and unlocalized outliers, resulting typically in a non-integrable field. The methods presented so far can only handle a small amount of outliers and noise due to the limited performance of their models. We present in this project a powerfull method for robust surface reconstruction. The proposed formulation is based on a triple sparsity prior : a sparse prior on the residual gradient field and a double sparse prior on the surface itself. A double prior corrects the outliers in the field, while the third sparsity prior smooths the surface to reduce the noise. We develop an efficient alternate minimization strategy to solve the proposed optimization problem. The method is able to recover a good quality surface from severely corrupted gradients thanks to its ability to handle both noise and outliers. We demonstrate the performance of the proposed method on synthetic and real data. Experiments show that the proposed solution outperforms some existing methods in the three possible cases : noise only, outliers only and mixed noise/outliers. See figure 9 .

Work submitted to CVPR 2014.

(a) Ground-truth (b) Diffusion (ECCV 2006) (c) l_1-norm (CVPR09) (d) Proposed

Figure 9. Photometric stereo reconstruction from noisy images. The proposed method produces amuch better reconstruction compared to two state-of-the-art methods.

MISTIS Project-Team

6. New Results

6.1. Mixture models

6.1.1. Parameter estimation in the heterogeneity linear mixed model

Participant: Marie-José Martinez.

Joint work with: Emma Holian (National University of Ireland, Galway)

In studies where subjects contribute more than one observation, such as in longitudinal studies, linear mixed models have become one of the most used techniques to take into account the correlation between these observations. By introducing random effects, mixed models allow the within-subject correlation and the variability of the response among the different subjects to be taken into account. However, such models are based on a normality assumption for the random effects and reflect the prior belief of homogeneity among all the subjects. To relax this strong assumption, Verbeke and Lesaffre (1996) proposed the extension of the classical linear mixed model by allowing the random effects to be sampled from a finite mixture of normal distributions with common covariance matrix. This extension naturally arises from the prior belief of the presence of unobserved heterogeneity in the random effects population. The model is therefore called the heterogeneity linear mixed model. Note that this model does not only extend the assumption about the random effects distribution, indeed, each component of the mixture can be considered as a cluster containing a proportion of the total population. Thus, this model is also suitable for classification purposes.

Concerning parameter estimation in the heterogeneity model, the use of the EM-algorithm, which takes into account the incomplete structure of the data, has been considered in the literature. Unfortunately, the M-step in the estimation process is not available in analytic form and a numerical maximisation procedure such as Newton-Raphson is needed. Because deriving such a procedure is a non-trivial task, Komarek et al. (2002) proposed an approximate optimization. But this procedure proved to be very slow and limited to small samples due to requiring manipulation of very large matrices and prohibitive computation.

To overcome this problem, we have proposed in [28], [52] an alternative approach which consists of fitting directly an equivalent mixture of linear mixed models. Contrary to the heterogeneity model, the M-step of the EM-algorithm is tractable analytically in this case. Then, from the obtained parameter estimates, we can easily obtain the parameter estimates in the heterogeneity model.

6.1.2. Taking into account the curse of dimensionality

Participants: Stéphane Girard, Alessandro Chiancone, Seydou-Nourou Sylla.

Joint work with: C. Bouveyron (Univ. Paris 1), M. Fauvel (ENSAT Toulouse) and J. Chanussot (Gipsa-lab and Grenoble-INP)

In the PhD work of Charles Bouveyron (co-advised by Cordelia Schmid from the Inria LEAR team) [64], we propose new Gaussian models of high dimensional data for classification purposes. We assume that the data live in several groups located in subspaces of lower dimensions. Two different strategies arise:

- the introduction in the model of a dimension reduction constraint for each group
- the use of parsimonious models obtained by imposing to different groups to share the same values of some parameters

This modelling yields a new supervised classification method called High Dimensional Discriminant Analysis (HDDA) [4]. Some versions of this method have been tested on the supervised classification of objects in images. This approach has been adapted to the unsupervised classification framework, and the related method is named High Dimensional Data Clustering (HDDC) [3]. Our recent work consists in adding a kernel in the previous methods to deal with nonlinear data classification.

6.1.3. Mixture modelling using skewed multivariate heavy tailed distributions with variable amounts of tailweight

Participants: Florence Forbes, Darren Wraith.

Clustering concerns the assignment of each of N, possibly multidimensional, observations $y_1, ..., y_N$ to one of K groups. A popular way to approach this task is via a parametric finite mixture model. While the vast majority of the work on such mixtures has been based on Gaussian mixture models in many applications the tails of normal distributions are shorter than appropriate or parameter estimations are affected by atypical observations (outliers). The family of location and scale mixtures of Gaussians has the ability to generate a number of flexible distributional forms. It nests as particular cases several important asymmetric distributions like the Generalised Hyperbolic distribution. The Generalised Hyperbolic distribution in turn nests many other well known distributions such as the Normal Inverse Gaussian (NIG) whose practical relevance has been widely documented in the literature. In a multivariate setting, we propose to extend the standard location and scale mixture concept into a so called multiple scaled framework which has the advantage of allowing different tail and skewness behaviours in each dimension of the variable space with arbitrary correlation between dimensions. The approach builds upon, and develops further, previous work on scale mixtures of Gaussians [25]. Estimation of the parameters is provided via an EM algorithm with a particular focus on NIG distributions. Inference is then extended to cover the case of mixtures of such multiple scaled distributions for application to clustering. Assessments on simulated and real data confirm the gain in degrees of freedom and flexibility in modelling data of varying tail behaviour and directional shape.

6.1.4. High-Dimensional Regression with Gaussian Mixtures and Partially-Latent Response Variables

Participant: Florence Forbes.

Joint work with: Antoine Deleforge and Radu Horaud from the Inria Perception team.

In this work we address the problem of approximating high-dimensional data with a low-dimensional representation. We make the following contributions. We propose an inverse regression method which exchanges the roles of input and response, such that the low-dimensional variable becomes the regressor, and which is tractable. We introduce a mixture of locally-linear probabilistic mapping model that starts with estimating the parameters of inverse regression, and follows with inferring closed-form solutions for the forward parameters of the high-dimensional regression problem of interest. Moreover, we introduce a partially-latent paradigm, such that the vector-valued response variable is composed of both observed and latent entries, thus being able to deal with data contaminated by experimental artifacts that cannot be explained with noise models. The proposed probabilistic formulation could be viewed as a latent-variable augmentation of regression. We devise expectation-maximization (EM) procedures based on a data augmentation strategy which facilitates the maximum-likelihood search over the model parameters. We propose two augmentation schemes and we describe in detail the associated EM inference procedures that may well be viewed as generalizations of a number of EM regression, dimension reduction, and factor analysis algorithms. The proposed framework is validated with both synthetic and real data. We provide experimental evidence that our method outperforms several existing regression techniques.

6.1.5. Acoustic space learning via variational EM for Sound-Source Separation and Localization

Participant: Florence Forbes.

Joint work with: Antoine Deleforge and Radu Horaud from the Inria Perception team.

In this paper we address the problems of modeling the acoustic space generated by a full-spectrum sound source and of using the learned model for the localization and separation of multiple sources that simultaneously emit sparse-spectrum sounds. We lay theoretical and methodological grounds in order to introduce the *binaural manifold* paradigm. We perform an in-depth study of the latent low-dimensional structure of the high-dimensional interaural spectral data, based on a corpus recorded with a human-like audiomotor robot head. A

non-linear dimensionality reduction technique is used to show that these data lie on a two-dimensional (2D) smooth manifold parameterized by the motor states of the listener, or equivalently, the sound source directions. We propose a *probabilistic piecewise affine mapping* model (PPAM) specifically designed to deal with high-dimensional data exhibiting an intrinsic piecewise linear structure. We derive a closed-form expectation-maximization (EM) procedure for estimating the model parameters, followed by Bayes inversion for obtaining the full posterior density function of a sound source direction. We extend this solution to deal with missing data and redundancy in real world spectrograms, and hence for 2D localization of natural sound sources such as speech. We further generalize the model to the challenging case of multiple sound sources and we propose a variational EM framework. The associated algorithm, referred to as *variational EM for source separation and localization* (VESSL) yields a Bayesian estimation of the 2D locations and time-frequency masks of all the sources. Comparisons of the proposed approach with several existing methods reveal that the combination of acoustic-space learning with Bayesian inference enables our method to outperform state-of-the-art methods.

6.2. Statistical models for Neuroscience

6.2.1. Hemodynamically informed parcellation of cerebral fMRI data

Participants: Florence Forbes, Aina Frau-Pascual, Thomas Vincent.

Joint work with: Philippe Ciuciu from Team Parietal and Neurospin, CEA in Saclay.

Standard detection of evoked brain activity in functional MRI (fMRI) relies on a fixed and known shape of the impulse response of the neurovascular coupling, namely the hemodynamic response function (HRF). To cope with this issue, the joint detection-estimation (JDE) framework has been proposed. This formalism enables to estimate a HRF per region but for doing so, it assumes a prior brain partition (or parcellation) regarding hemodynamic territories (eg. [14]). This partition has to be accurate enough to recover accurate HRF shapes but has also to overcome the detection-estimation issue: the lack of hemodynamics information in the non-active positions. During the internship of A. Frau Pascual at Neurospin, we proposed an hemodynamically-based parcellation, consisting first of a feature extraction step, followed by a Gaussian Mixture-based parcellation, which considers the injection of the activation levels in the parcellation process, in order to overcome the detection-estimation issue and find the underlying hemodynamics. The work has been submitted to the ICASSP conference in 2014.

6.2.2. Variational variable selection to assess experimental condition relevance in event-related fMRI

Participants: Florence Forbes, Christine Bakhous, Lotfi Chaari, Thomas Vincent, Farida Enikeeva.

Joint work with: Michel Dojat (Grenoble Institute of Neuroscience) and Philippe Ciuciu from Neurospin, CEA in Saclay.

Brain functional exploration investigates the nature of neural processing following cognitive or sensory stimulation. This goal is not fully accounted for in most functional Magnetic Resonance Imaging (fMRI) analysis which usually assumes that all delivered stimuli possibly generate a BOLD response everywhere in the brain although activation is likely to be induced by only some of them in specific brain regions. Generally, criteria are not available to select the relevant conditions or stimulus types (e.g. visual, auditory, etc.) prior to activation detection and the inclusion of irrelevant events may degrade the results, particularly when the Hemodynamic Response Function (HRF) is jointly estimated as in the JDE framework mentioned in the previous section. To face this issue, we propose an efficient variational procedure that automatically selects the conditions according to the brain activity they elicit. It follows an improved activation detection and local HRF estimation that we illustrate on synthetic and real fMRI data. This approach is an alternative to our previous approach based on Monte-Carlo Markov Chain (MCMC) inference [63]. Corresponding papers [31], [45]. A synthesis can also be found in the PhD manuscript of C. Bakhous (Grenoble University, December 2013) [11].

6.2.3. Bayesian Joint Detection-Estimation of cerebral vasoreactivity from ASL fMRI data

Participants: Florence Forbes, Thomas Vincent.

In the context of ARC AINSI project, joint work with: Philippe Ciuciu from Neurospin, CEA in Saclay.

Functional MRI (fMRI) is the method of choice to non-invasively probe cerebral activity evoked by a set of controlled experimental conditions. A rising fMRI modality is Arterial Spin Labeling (ASL) which enables to quantify the cerebral perfusion, namely the cerebral blood flow (CBF) and emerges as a more direct biomarker of neuronal activity than the standard BOLD (Blood Oxygen Level Dependent) fMRI.

Although the study of cerebral vasoreactivity using fMRI is mainly conducted through the BOLD fMRI modality (see the two previous sections), owing to its relatively high signal-to-noise ratio (SNR), ASL fMRI provides a more interpretable measure of cerebral vasoreactivity than BOLD fMRI. Still, ASL suffers from a low SNR and is hampered by a large amount of physiological noise. Our contribution, described in [43], [44] aims at improving the recovery of the vasoreactive component from the ASL signal. To this end, a Bayesian hierarchical model is proposed, enabling the recovery of perfusion levels as well as fitting their dynamics. On a single-subject ASL real data set involving perfusion changes induced by hypercapnia, the approach is compared with a classical GLM-based analysis. A better goodness-of-fit is achieved, especially in the transitions between baseline and hypercapnia periods. Also, perfusion levels are recovered with higher sensitivity and show a better contrast between gray- and white matter.

6.2.4. Physiologically-inspired Bayesian analysis of BOLD and ASL fMRI data

Participants: Florence Forbes, Thomas Vincent, Jennifer Sloboda.

In the context of ARC AINSI project, joint work with: Philippe Ciuciu from Neurospin, CEA in Saclay.

The ASL modality is most commonly used as a static measure where the average perfusion is computed over a volume sequence lasting several minutes. Recently, ASL has been used in functional activation protocols and hence gives access to a dynamic measure of perfusion, namely the variations of CBF which are elicited by specific tasks. ASL MRI mainly consists of acquiring pairs of control and label images and looking at the average control-label difference. The Signal-to-Noise Ratio (SNR) of this difference is very low so that several hundreds of image pairs need to be acquired, thus increasing significantly the time spent by the subject in the scanner and making the acquisition very sensitive to the patient's movement. In addition, this averaging requires that the perfusion signal is at a steady state, limiting the scope of fMRI task experiments to baseline perfusion measurements or long block designs. In contrast, it is highly desirable to measure change in perfusion due to an effect of interest in activation paradigms from event-related designs. It is technically possible to collect event-related ASL data but most approaches to functional ASL data analysis use a standard linear model (GLM-based) formulation with regressors encoding differences in control/tag scans and both ASL and BOLD activation signals being associated with the same canonical response function. The canonical hemodynamic response function (HRF) is generally used although it has been been calibrated on BOLD experiments only, thus reflecting simultaneous variations of CBF, cerebral blood volume (CBV) and cerebral oxygen consumption (CMRO2). In contrast, the perfusion signal only reflects variation in CBF so that the associated response, the perfusion response function (PRF), is likely to differ from the HRF. In the internship proposal of Jennifer Sloboda, we proposed to recover both a hemodynamic (BRF for BOLD response function) and a perfusion (PRF) response functions from event-related functional ASL data. To do so, a joint detection estimation (JDE) formalism was used. In the BOLD context, the JDE framework has proven to successfully extract the HRF while also performing activation detection. We had recently extended this formalism (see Section 6.2.3 and [43], [44]) to model an additional perfusion component linked to the BOLD one through a common activation detection. The main issue addressed then was to characterize the link between BOLD and perfusion components. To establish this link, we proposed a methodological axis which consists of developing a physiologically-inspired approach. To do so, dynamical non-linear equations available in physiological models were linearized and approximated in a parsimonious way so as to establish prior relations between the perfusion and BOLD responses which can be injected in our Bayesian setting. The inference of the initial model is currently done through a Markov Chain Monte Carlo approach but a Variational Expectation-Maximization implementation is also conceivable. As such, the tasks were two-fold: (1) investigate the physiological model and (2) inject it into the JDE setting. Investigation of the physiological model allows for: (1) creation of artificial fMRI data, (2) investigation of the relationship between physiological changes

and the resulting simulated BOLD or ASL signal, and (3) characterization of the link between BOLD and perfusion responses. Injection of the physiologically inspired prior into the JDE model, is to (1) improve perfusion response recovery, (2) determine physiologically quantified units to the JDE recovered values This work is going to serve as a preliminary investigation into the incorporation of physiological information in the Bayesian JDE setting from which to determine the trajectory of future model developments.

6.3. Markov models

6.3.1. Spatial modelling of plant diversity from high-throughput environmental DNA sequence data

Participants: Florence Forbes, Angelika Studeny.

This is joint work with: Eric Coissac and Pierre Taberlet from LECA (Laboratoire d'Ecologie Alpine) and Alain Viari from Inria team Bamboo.

This work [48] considers a statistical modelling approach to investigate spatial cross-correlations between species in an ecosystem. A special feature is the origin of the data from high-troughput environmental DNA sequencing of soil samples. Here we use data collected at the Nouragues CNRS Field Station in French Guiana. We describe bivariate spatial relationships in these data by a separable linear model of coregionalisation and estimate a cross-correlation parameter. Based on this estimate, we visualise plant taxa co-occurrence pattern in form of 'interaction graphs' which can be interpreted in terms of ecological interactions. Limitations of this approach are discussed along with possible alternatives in [48].

6.3.2. Modelling multivariate counts with graphical Markov models.

Participants: Jean-Baptiste Durand, Florence Forbes, Marie-José Martinez, Angelika Studeny.

Joint work with: Pierre Fernique (Montpellier 2 University, CIRAD and Inria Virtual Plants), Yann Guédon (CIRAD and Inria Virtual Plants) and Iragaël Joly (INRA-GAEL and Grenoble INP).

Multivariate count data are defined as the number of items of different categories issued from sampling within a population, which individuals are grouped into categories. The analysis of multivariate count data is a recurrent and crucial issue in numerous modelling problems, particularly in the fields of biology and ecology (where the data can represent, for example, children counts associated with multitype branching processes), sociology and econometrics. Denoting by K the number of categories, multivariate count data analysis relies on modelling the joint distribution of the K-dimensional random vector $N = (N_0, ..., N_{K-1})$ with discrete components. Our work focused on I) Identifying categories that appear simultaneously, or on the contrary that are mutually exclusive. This was achieved by identifying conditional independence relationships between the K variables; II)Building parsimonious parametric models consistent with these relationships; III) Characterizing and testing the effects of covariates on the distribution of N, particularly on the dependencies between its components.

Our context of application was characterised by zero-inflated, often right skewed marginal distributions. Thus, Gaussian and Poisson distributions were not *a priori* appropriate. Moreover, the multivariate histograms typically had many cells, most of which were empty. Consequently, nonparametric estimation was not efficient.

To achieve these goals, we proposed an approach based on graphical probabilistic models (Koller & Friedman, 2009 [70]) to represent the conditional independence relationships in N, and on parametric distributions to ensure model parsimony [51]. The considered graphs were partially directed, so as to represent both marginal independence relationships and cyclic dependencies between quadruplets of variables (at least).

Graph search was achieved by a stepwise approach, issued from unification of previous algorithms presented in Koller & Friedman (2009) for DAGs: Hill climbing, greedy search, first ascent and simulated annealing. The search algorithm was improved by taking into account our parametric distribution assumptions, which led to caching overlapping graphs at each step. An adaptation to PDAGs of graph search algorithms for DAGs was developed, by defining new operators specific to PDAGs.

Comparisons between different algorithms in the literature for directed and undirected graphical models was performed on simulated datasets to: (i) Assess gain in speed induced by caching; (ii) Compare the graphs obtained under parametric and nonparametric distributions assumptions; (iii) Compare different strategies for graph initialization. Strategies based on several random graphs were compared to those based on a fast estimation of an undirected graph, assumed to be the moral graph.

First results were obtained in modelling individual daily activity program [50] and interactions between flowering and vegetative growth in plants (see sections below).

6.3.3. *Statistical characterization of tree structures based on Markov tree models and multitype branching processes, with applications to tree growth modelling.*

Participant: Jean-Baptiste Durand.

Joint work with: Pierre Fernique (Montpellier 2 University and CIRAD) and Yann Guédon (CIRAD), Inria Virtual Plants.

The quantity and quality of yields in fruit trees is closely related to processes of growth and branching, which determine ultimately the regularity of flowering and the position of flowers. Flowering and fruiting patterns are explained by statistical dependence between the nature of a parent shoot (*e.g.* flowering or not) and the quantity and natures of its children shoots – with potential effect of covariates. Thus, better characterization of patterns and dependences is expected to lead to strategies to control the demographic properties of the shoots (through varietal selection or crop management policies), and thus to bring substantial improvements in the quantity and quality of yields.

Since the connections between shoots can be represented by mathematical trees, statistical models based on multitype branching processes and Markov trees appear as a natural tool to model the dependencies of interest. Formally, the properties of a vertex are summed up using the notion of vertex state. In such models, the numbers of children in each state given the parent state are modeled through discrete multivariate distributions. Model selection procedures are necessary to specify parsimonious distributions. We developed an approach based on probabilistic graphical models (see Section 6.3.2) to identify and exploit properties of conditional independence between numbers of children in different states, so as to simplify the specification of their joint distribution [51], [32].

This work was carried out in the context of Pierre Fernique's first year of PhD (Montpellier 2 University and CIRAD). It was applied to model dependencies between short or long, vegetative or flowering shoots in apple trees. The results highlighted contrasted patterns related to the parent shoot state, with interpretation in terms of alternation of flowering (see paragraph 6.3.4). It was also applied to the analysis of the connections between cyclic growth and flowering of mango trees [32]. This work will be continued during Pierre Fernique's PhD thesis, with extensions to other fruit tree species and other parametric discrete multivariate families of distributions, including covariates and mixed effects.

6.3.4. *Statistical characterization of the alternation of flowering in fruit tree species*

Participant: Jean-Baptiste Durand.

Joint work with: Jean Peyhardi and Yann Guédon (Mixed Research Unit DAP, Virtual Plants team), Baptiste Guitton, Yan Holtz and Evelyne Costes (DAP, AFEF team), Catherine Trottier (Montpellier University)

A first study was performed to characterize genetic determinisms of the alternation of flowering in apple tree progenies [37], [21]. Data were collected at two scales: at whole tree scale (with annual time step) and a local scale (annual shoot or AS, which is the portions of stem that were grown during the same year). Two replications of each genotype were available.

Indices were proposed to characterize alternation at tree scale. The difficulty is related to early detection of alternating genotypes, in a context where alternation is often concealed by a substantial increase of the number of flowers over consecutive years. To separate correctly the increase of the number of flowers due to aging of young trees from alternation in flowering, our model relied on a parametric hypothesis for the trend (fixed slopes specific to genotype and random slopes specific to replications), which translated into mixed effect

modelling. Then, different indices of alternation were computed on the residuals. Clusters of individuals with contrasted patterns of bearing habits were identified.

To model alternation of flowering at AS scale, a second-order Markov tree model was built. Its transition probabilities were modelled as generalized linear mixed models, to incorporate the effects of genotypes, year and memory of flowering for the Markovian part, with interactions between these components.

Asynchronism of flowering at AS scale was assessed using an entropy-based criterion. The entropy allowed for a characterisation of the roles of local alternation and asynchronism in regularity of flowering at tree scale.

Moreover, our models highlighted significant correlations between indices of alternation at AS and individual scales.

This work was extended by the Master 2 internship of Yan Holtz, supervised by Evelyne Costes and Jean-Baptiste Durand. New progenies were considered, and a methodology based on a lighter measurement protocol was developed and assessed. It consisted in assessing the accuracy of approximating the indices computed from measurements at tree scale by the same indices computed as AS scale. The approximations were shown sufficiently accurate to provide an operational strategy for apple tree selection.

As a perspective of this work, patterns in the production of children ASs (numbers of flowering and vegetative children) depending on the type of the parent AS must be analyzed using branching processes and different types of Markov trees, in the context of Pierre Fernique's PhD Thesis (see paragraph 6.3.3).

6.4. Semi and non-parametric methods

6.4.1. Modelling extremal events

Participants: Stéphane Girard, El-Hadji Deme.

Joint work with: L. Gardes (Univ. Strasbourg) and E. Deme (Univ. Gaston Berger, Sénégal)

We are working on the estimation of the second order parameter ρ (see paragraph 3.3.1). We proposed a new family of estimators encompassing the existing ones (see for instance [69], [68]). This work is in collaboration with El-Hadji Deme who obtained a grant (IBNI price) to work within the Mistis team on extreme-value statistics. The results are published in [18].
In addition to this work, we have established a review on the Weibull-tail distributions [29].

6.4.2. Conditional extremal events

Participants: Stéphane Girard, Gildas Mazo, Jonathan El-Methni.

Joint work with: L. Gardes (Univ. Strasbourg) and A. Daouia (Univ. Toulouse I and Univ. Catholique de Louvain)

The goal of the PhD thesis of Alexandre Lekina was to contribute to the development of theoretical and algorithmic models to tackle conditional extreme value analysis, *ie* the situation where some covariate information X is recorded simultaneously with a quantity of interest Y. In such a case, the tail heaviness of Y depends on X, and thus the tail index as well as the extreme quantiles are also functions of the covariate. We combine nonparametric smoothing techniques [66] with extreme-value methods in order to obtain efficient estimators of the conditional tail index and conditional extreme quantiles. When the covariate is functional and random (random design) we focus on kernel methods [16].

Conditional extremes are studied in climatology where one is interested in how climate change over years might affect extreme temperatures or rainfalls. In this case, the covariate is univariate (time). Bivariate examples include the study of extreme rainfalls as a function of the geographical location. The application part of the study is joint work with the LTHE (Laboratoire d'étude des Transferts en Hydrologie et Environnement) located in Grenoble.

6.4.3. Estimation of extreme risk measures

Participants: Stéphane Girard, Jonathan El-Methni, El-Hadji Deme.

Joint work with: L. Gardes and A. Guillou (Univ. Strasbourg)

One of the most popular risk measures is the Value-at-Risk (VaR) introduced in the 1990's. In statistical terms, the VaR at level $\alpha \in (0,1)$ corresponds to the upper α-quantile of the loss distribution. The Value-at-Risk however suffers from several weaknesses. First, it provides us only with a pointwise information: VaR(α) does not take into consideration what the loss will be beyond this quantile. Second, random loss variables with light-tailed distributions or heavy-tailed distributions may have the same Value-at-Risk . Finally, Value-at-Risk is not a coherent risk measure since it is not subadditive in general. A coherent alternative risk measure is the Conditional Tail Expectation (CTE), also known as Tail-Value-at-Risk, Tail Conditional Expectation or Expected Shortfall in case of a continuous loss distribution. The CTE is defined as the expected loss given that the loss lies above the upper α-quantile of the loss distribution. This risk measure thus takes into account the whole information contained in the upper tail of the distribution. It is frequently encountered in financial investment or in the insurance industry. In [36], we have established the asymptotic properties of the classical CTE estimator in case of extreme losses, *i.e.* when $\alpha \to 0$ as the sample size increases. We have exhibited the asymptotic bias of this estimator, and proposed a bias correction based on extreme-value techniques [36]. Similar developments have been achieved in the case of the Proportional Hazard Premium measure of risk [19]. In [22], we study the situation where some covariate information is available. We thus has to deal with conditional extremes (see paragraph 6.4.2). We also proposed a new risk measure (called the Conditional Tail Moment) which encompasses various risk measures, such as the CTE, as particular cases.

6.4.4. Multivariate extremal events

Participants: Stéphane Girard, Gildas Mazo, Florence Forbes, Van Trung Pham.

Joint work with: C. Amblard (TimB in TIMC laboratory, Univ. Grenoble I) and L. Menneteau (Univ. Montpellier II)

Copulas are a useful tool to model multivariate distributions [72]. At first, we developed an extension of some particular copulas [1]. It followed a new class of bivariate copulas defined on matrices [56] and some analogies have been shown between matrix and copula properties.

However, while there exist various families of bivariate copulas, much fewer has been done when the dimension is higher. To this aim an interesting class of copulas based on products of transformed copulas has been proposed in the literature. The use of this class for practical high dimensional problems remains challenging. Constraints on the parameters and the product form render inference, and in particular the likelihood computation, difficult. We proposed a new class of high dimensional copulas based on a product of transformed bivariate copulas [61]. No constraints on the parameters refrain the applicability of the proposed class which is well suited for applications in high dimension. Furthermore the analytic forms of the copulas within this class allow to associate a natural graphical structure which helps to visualize the dependencies and to compute the likelihood efficiently even in high dimension. The extreme properties of the copulas are also derived and an R package has been developed.

As an alternative, we also proposed a new class of copulas constructed by introducing a latent factor. Conditional independence with respect to this factor and the use of a nonparametric class of bivariate copulas lead to interesting properties like explicitness, flexibility and parsimony. In particular, various tail behaviours are exhibited, making possible the modeling of various extreme situations. A pairwise moment-based inference procedure has also been proposed and the asymptotic normality of the corresponding estimator has been established [53].

6.4.5. Level sets estimation

Participant: Stéphane Girard.

Joint work with: A. Guillou and L. Gardes (Univ. Strasbourg), G. Stupfler (Univ. Aix-Marseille) and A. Daouia (Univ. Toulouse I and Univ. Catholique de Louvain)

The boundary bounding the set of points is viewed as the larger level set of the points distribution. This is then an extreme quantile curve estimation problem. We proposed estimators based on projection as well as on kernel regression methods applied on the extreme values set, for particular set of points [10]. We also investigate the asymptotic properties of existing estimators when used in extreme situations. For instance, we have established in collaboration with G. Stupfler that the so-called geometric quantiles have very counter-intuitive properties in such situations [60] and thus should not be used to detect outliers.
In collaboration with A. Daouia, we investigate the application of such methods in econometrics [17]: A new characterization of partial boundaries of a free disposal multivariate support is introduced by making use of large quantiles of a simple transformation of the underlying multivariate distribution. Pointwise empirical and smoothed estimators of the full and partial support curves are built as extreme sample and smoothed quantiles. The extreme-value theory holds then automatically for the empirical frontiers and we show that some fundamental properties of extreme order statistics carry over to Nadaraya's estimates of upper quantile-based frontiers.
In collaboration with G. Stupfler and A. Guillou, new estimators of the boundary are introduced. The regression is performed on the whole set of points, the selection of the "highest" points being automatically performed by the introduction of high order moments [26], [27].

6.4.6. Retrieval of Mars surface physical properties from OMEGA hyperspectral images.

Participants: Stéphane Girard, Alessandro Chiancone.

Joint work with: S. Douté from Laboratoire de Planétologie de Grenoble, J. Chanussot (Gipsa-lab and Grenoble-INP) and J. Saracco (Univ. Bordeaux).

Visible and near infrared imaging spectroscopy is one of the key techniques to detect, to map and to characterize mineral and volatile (eg. water-ice) species existing at the surface of planets. Indeed the chemical composition, granularity, texture, physical state, etc. of the materials determine the existence and morphology of the absorption bands. The resulting spectra contain therefore very useful information. Current imaging spectrometers provide data organized as three dimensional hyperspectral images: two spatial dimensions and one spectral dimension. Our goal is to estimate the functional relationship F between some observed spectra and some physical parameters. To this end, a database of synthetic spectra is generated by a physical radiative transfer model and used to estimate F. The high dimension of spectra is reduced by Gaussian regularized sliced inverse regression (GRSIR) to overcome the curse of dimensionality and consequently the sensitivity of the inversion to noise (ill-conditioned problems) [57]. We have also defined an adaptive version of the method which is able to deal with block-wise evolving data streams [15].

6.4.7. High-dimensional change-point detection with sparse alternatives

Participant: Farida Enikeeva.

Joint work with: Zaid Harchaoui from LEAR team Inria Grenoble

The change-point problem is a classical problem of statistics that arises in various applications as signal processing, bioinformatics, financial market analysis. The goal of change-point problems is to make an inference about the moment of a change in the distribution of the observed data. We consider the problem of detection of a simultaneous change in mean in a sequence of Gaussian vectors.

The state-of-the-art approach to the change-point detection/estimation is based on the assumption of growing number of observations and fixed dimension of the signal. We work in high-dimensional setting assuming that the vector dimension tends to infinity and the length of the sequence grows slower than the dimension of the signal. Assuming that the change occurs only in a subset of the vector components of unknown cardinality we can reduce our problem to the problem of testing non-zero components in a sequence of sparse Gaussian vectors. We construct a testing procedure that is adaptive to the number of components with a change. This testing procedure is based on combination of two chi-squared type test statistics. This combined test provides an optimal performance of the test both in the cases of high and moderate sparsity. We obtain the detection boundary of the test and show its rate-optimality in minimax sense.

The results of the paper [59] were presented at

- NIPS 2013, Workshop on Modern Nonparametric Methods in Machine Learning (Dec. 2013)
- Conference on Structural Inference in Statistics, Potsdam, Germany (Sept. 2013)

6.4.8. Yield Improvement by the Redundancy Method for Component Calibration

Participant: Farida Enikeeva.

Joint work with: Dominique Morche (CEA-LETI) and Alp Oguz (CEA-LETI)

This work [23] was done in the framework of the Optimyst II project of MINALOGIC in collaboration with CEA-LETI and LJK-UJF. In this project we explore the benefits of the redundant channels methodology for the calibration of electronic components.

The demand for high data rate in communication puts stringent requirements on components' dynamic range. However, the extreme size reduction in advanced technology results inadvertently in increased process variability, which inherently limits the performances. The redundancy approach is based on the idea of dividing an elementary component (capacitor, resistor, transistor) into several subsets and then choosing an optimal combination of such subsets to provide the production of a component with very precise characteristics. For several years, the redundancy method has been identified as complementary to digital calibration to improve the performances. On practice, it is hard for a designer to select an optimal number of redundant components to provide the desired production yield and to minimize the area occupied by the components. The usual way to solve this problem is to resort to statistical simulations which are time consuming and sometimes misleading. We propose a normal approximation of the yield in order to estimate the number of redundant components needed to provide a minimal area occupied by the components.

MODAL Project-Team

6. New Results

6.1. Resampling procedures

Participant: Alain Celisse.

The new deep understanding of cross-validation procedures in density estimation has been tackled with new results in terms of risk estimation and model selection [7]. This is the first step towards a fully data-driven and optimal choice of cross-validation strategy.

6.2. Kernel change-point

Participants: Alain Celisse, Guillemette Marot, Morgane Pierre-Jean.

On the basis of theoretical arguments, an empirical analysis has been carried out to assess the influence of the choice of the kernel in the kernel change-point strategy described in [2]. This assessment has been done in the biological context of copy number variation and allele B fraction. Several talks have been given in seminars (SSB seminar in Paris,...) and workshops (JSFDS, SMPGD,...)

6.3. Gaussian process in RKHS

Participants: Alain Celisse, Jérémie Kellner.

Since numerous papers make a Gaussian assumption for observations in the reproducing kernel Hilbert space (RKHS), it is important to be able to assess the validity of this crucial assumption. As long as it has been validated, the Gaussian framework can be further used to infer statistical properties of the population at hand (mean, variance,...).

A statistical test has been designed to address such questions at the RKHS level. It is fully computationally efficient and provides really good power in numerous settings. Theoretical properties for the test statistic have been derived as well.

6.4. Model for conditionally correlated categorical data

Participants: Christophe Biernacki, Matthieu Marbac-Lourdelle, Vincent Vandewalle.

It is a model-based clustering where categorical data are grouped into conditionally independent blocks. The corresponding block distribution is a parsimonious multinomial distribution where the few free parameters correspond to the most likely modality crossings, while the remaining probability mass is uniformly spread over the other modality crossings. The exact computation of the integrated complete-data likelihood allows to perform the model selection, by a Gibbs sampler, reducing the computing time consuming by parameter estimation and avoiding BIC criterion biases pointed out by our experiments.

This model was presented in a conference [13] with scientific committee and in a seminar [17]. An article will be soon submitted. Furthermore, a R package is currently under development.

6.5. Mixture model for mixed kind of data

Participants: Christophe Biernacki, Matthieu Marbac-Lourdelle, Vincent Vandewalle.

A mixture model of Gaussian copula allows to cluster mixed kind of data. Each component is composed by classical margins while the conditional dependencies between the variables is modeled by a Gaussian copula. The parameter estimation is performed by a Gibbs sampler. This model was presented in a conference [14]. Some technical points will be developed before providing an article.

6.6. Mixture of Gaussians with Missing Data

Participants: Christophe Biernacki, Vincent Vandewalle.

The generative models allow to handle missing data. This can be easily performed by using the EM algorithm, which has a closed form M-step in the Gaussian setting. This can for instance be useful for distance estimation with missing data. It has been proposed to improve the distance estimation by fitting a mixture of Gaussian distributions instead of a considering only one Gaussian component [21]. This is a joined work with Emil Eirola and Amaury Lendrasse .

A parallel work is in progress on the mixture degeneracy when considering mixture of Gaussians with missing data. It have been experimentally noticed that the degeneracy in this case is particularly slow. This behaviour is different from the usual setting of degeneracy with mixture of Gaussians which is usually rather fast. A first attempt of the theoretical characterization of this behaviour around a degenerated solution has been presented at a conference [16].

6.7. Transfert learning in model-based clustering

Participant: Christophe Biernacki.

In many situations one needs to cluster several datasets, possibly arising from different populations, instead of a single one, into partitions with identical meaning and described by similar features. Such situations involve commonly two kinds of standard clustering processes. The samples are clustered traditionally either as if all units arose from the same distribution, or on the contrary as if the samples came from distinct and unrelated populations. But a third situation should be considered: As the datasets share statistical units of same nature and as they are described by features of same meaning, there may exist some link between the samples. We propose a linear stochastic link between the samples, what can be justified from some simple but realistic assumptions, both in the Gaussian and in the t mixture model-based clustering context [26]. This is a joint work with Alexandre Lourme.

6.8. Gaussian Models Scale Invariant and Stable by Projection

Participant: Christophe Biernacki.

Gaussian mixture model-based clustering is now a standard tool to determine an hypothetical underlying structure into continuous data. However many usual parsimonious models, despite their appealing geometrical interpretation, suffer from major drawbacks as scale dependence or unsustainability of the constraints by projection. In this work we present a new family of parsimonious Gaussian models based on a variance-correlation decomposition of the covariance matrices. These new models are stable by projection into the canonical planes and, so, faithfully representable in low dimension. They are also stable by modification of the measurement units of the data and such a modification does not change the model selection based on likelihood criteria. We highlight all these stability properties by a specific geometrical representation of each model. A detailed GEM algorithm is also provided for every model inference. Then, on biological and geological data, we compare our stable models to standard geometrical ones.

This joint work with Alexandre Lourme is now published in [6].

6.9. Clustering and variable selection in regression

Participants: Christophe Biernacki, Loïc Yengo, Julien Jacques.

A new framework is proposed to address the issue of simultaneous linear regression and clustering of predictors where regression coefficients are assumed to be drawn from a Gaussian mixture distribution. Prediction is thus performed using the conditional distribution of the regression coefficients given the data, while clusters are easily derived from posterior distribution in groups given the data. This work is now published in [28]

6.10. An AIC-like criterion for semi-supervised classification

Participants: Christophe Biernacki, Vincent Vandewalle.

In semi-supervised classification, generative models take naturally into account unlabeled data and parameter estimation can be easily performed through the EM algorithm. However, traditional model selection criteria either does not take into consideration the predictive purpose (AIC or BIC criteria) or involve a high computational cost because of the EM mechanism (cross validation criteria). Alternatively, we propose the penalized model selection criterion AICcond which aims to estimate the predictive power of a generative model by approximating its predictive deviance. AICcond has similar computational cost to AIC, owns good consistency theoretical properties and highlights encouraging behaviour for variable and model selection in comparison to other standard criteria.

This joint work with Gilles Celeux and Gérard Govaert is now published in[16].

6.11. Consistency of a nonparametric conditional mode estimator for random fields

Participant: Sophie Dabo-Niang.

Sophie Dabo-Niang settled the consistency of a nonparametric conditional mode estimator for random fields, Statistical Methods and Applications [9].

6.12. Spatial linear models

Spatial linear models only capture global linear relationships between locations. However, in many circumstances the spatial dependency is not linear. It is, for example, the classical case where one deals with the spatial pattern of extreme events such as in the economic analysis of poverty, in the environmental science,... This leads naturally to consider nonparametric modeling.

6.13. Auto-associative models

Serge Iovleff gave a complete treatment of the Auto-Associative models in the semi-linear case and wrote a software for estimating these models (hal-00734070, version 1).

6.14. BlockCluster

Serge Iovleff has submitted a paper on the BlockCluster package in collaboration with Parmeet Bathia.

6.15. Rmixmod

Serge Iovleff has contributed to a paper submitted to JSS (hal-00919486, version 1) in collaboration with R. Lebret, F. Langrognet, C. Biernacki, G. Celeux, and G. Govaert.

6.16. Clustering for functional data

Participants: Julien Jacques, Cristian Preda.

In Jacques & Preda 2014 (CSDA), we propose a model-based clustering algorithm for multivariate functional data, based on multivariate functional principal components analysis. A review on clustering for functional data has also be published in Jacques & Preda 2014 (ADAC). Variable selection in high-dimensional regression Participants: Julie Hamon, Julien Jacques, Clarisse Dhaenens. In the context of genomic analysis, dealing with high-throughput genotyping data, we develop a genetic algorithm which looks for the best subset of variables (of given size) to predict some quantitative feature.

6.17. Wavelet based clustering using mixed effects functional models

Participant: Guillemette Marot.

The paper related to the wavelet based clustering procedure presented in the activity report from MODAL team in 2012 was published in Biometrics [22].

6.18. Differential meta-analysis of RNA-seq data from multiple studies

Participant: Guillemette Marot.

An adaptation of meta-analysis methods intially proposed for microarray studies has been proposed for RNA-seq data. The R package metaRNASeq is available on the R Forge and the preprint of the paper is available on Arxiv [48].

6.19. Toxoplasma transcription factor TgAP2XI-5 regulates the expression of genes involved in parasite virulence and host invasion

Participant: Guillemette Marot.

The use of peak detection methods implemented in the Bioconductor package `Ringo` has enabled to better understand part of the gene regulation process in T. Gondii parasite. The new findings in Biology have been published in *Walker (2013)*.

REALOPT Project-Team

6. New Results

6.1. Extending the column generation paradigm

Building on our technical review [89] of methods for solving the Lagrangian Dual (with an analysis of the scope for hybridization) we have worked on methodologies that can be understood as an extension of the column generation approach in [22]. Working in an extended variable space allows one to develop tighter reformulations for mixed integer programs. To handle the size of the extended formulation, one can work with inner approximations defined and improved by generating dynamically variables and constraints. This so-called "column-and-row generation" procedure is revisited here in a unifying presentation that generalizes the column generation algorithm and extends to the case of working with an approximate extended formulation. A key benefit of this approach is that lifting pricing problem solutions in the space of the extended formulation permits their recombination into new subproblem solutions and results in faster convergence. The interest of the approach is evaluated numerically on machine scheduling, bin packing, generalized assignment, and multi-echelon lot-sizing problems. We compare a direct handling of the extended formulation, a standard column generation approach, and the “column-and-row generation” procedure. Within the Samba project we further showed that this stabilization offered by the recombination of solutions is complementary and adds up to stabilization techniques based on smoothing that were developed within Samba. These techniques have been applied in [26], [29].

6.2. Interior point cutting plane strategy revisited for column generation

In [89], we identify what are the stabilization features that are built into variants of subgradient algorithms and polyhedral approaches. In [27], we further compare their theoretical performance and discuss their combination. Stabilization procedures for column generation can be viewed as cutting plane strategies in the dual. Exploiting the link between in-out separation strategies and dual price smoothing techniques for column generation, we derive a generic bound convergence property for algorithms using a smoothing feature. Such property adds to existing in-out asymptotic convergence results. In our study on In-Out Separation and Column Generation Stabilization by Dual Price Smoothing, we note that our convergence property adds to existing in-out asymptotic convergence results. Beyond theoretically convergence, we describe in [88] a proposal for effective finite convergence in practice and we develop a smoothing auto-regulating strategy that makes the need for parameter tuning obsolete. Practical speed-up convergence that are observed go from 20% to 500 %. These contributions turn stabilization by smoothing into a general purpose practical scheme that can be used into a generic column generation procedure. We conclude the paper by showing that the approach can be combined with an ascent method, leading to improved performances. Such combination might inspire novel cut separation strategies.

6.3. A MILP approach to minimize the number of late jobs with and without machine availability constraints

The study in [13] investigates scheduling problems that occur when the weighted number of late jobs that are subject to deterministic machine availability constraints have to be minimized. These problems can be modeled as a more general job selection problem. Cases with resumable, non-resumable, and semi-resumable jobs as well as cases without availability constraints are investigated. The proposed efficient mixed integer linear programming approach includes possible improvements to the model, notably specialized lifted knapsack cover cuts. The method proves to be competitive compared with existing dedicated methods: numerical experiments on randomly generated instances show that all 350-job instances of the test bed are closed for the well-known problem $1|r_i|\sum w_i U_i$. For all investigated problem types, 98.4% of 500-job instances can be solved to optimality within one hour.

6.4. Multidimensional dual-feasible functions

Dual-feasible functions have been used in the past to compute lower bounds and valid inequalities for different combinatorial optimization and integer programming problems. Until now, all the dual-feasible functions proposed in the literature were 1-dimensional functions. In [11] we extended the principles of dual-feasible functions to the m-dimensional case by introducing the concept of vector packing dual-feasible function. We explored the theoretical properties of these functions in depth, and we proposed general schemes for generating some instances of these functions. Additionally, we proposed and analyzed different new families of vector packing dual-feasible functions. All the proposed approaches were tested extensively using benchmark instances of the 2-dimensional vector packing problem. Our computational results showed that these functions can approximate very efficiently the best lower bounds for this problem.

6.5. New branch-and-price methods for variants of bin packing problems

We proposed branch-and-price methods for two variants of the well-known bin-packing problem.

The bin packing problem with conflicts consists in packing items in a minimum number of bins of limited capacity while avoiding joint assignments of items that are in con ict. The study in [21] demonstrates that a generic implementation of a Branch-and-Price algorithm using specific pricing oracle yields comparatively good performance for this problem. We use our black-box Branch-and-Price solver BaPCod, relying on its generic branching scheme and primal heuristics. We developed a dynamic programming algorithm for pricing when the conflict graph is an interval graph, and a depth-first-search branch-and-bound approach for pricing when the conflict graph has no special structure. The exact method was tested on instances from the literature where the conflict graph is an interval graph, as well as harder instances that we generated with an arbitrarily conflict graph and larger number of items per bin. Our computational experiment report sets new benchmark results for this problem, closing all open instances of the literature in one hour of CPU time.

In the bin-packing with fragile objects, we are given a set of objects, each characterized by a weight and a fragility, and a large number of uncapacitated bins. Our aim is to find the minimum number of bins needed to pack all objects, in such a way that in each bin the sum of the object weights is less than or equal to the smallest fragility of an object in the bin. The problem is known in the literature as the Bin Packing Problem with Fragile Objects, and appears in the telecommunication field, when one has to assign cellular calls to available channels by ensuring that the total noise in a channel does not exceed the noise acceptance limit of a call. In [10], we propose a branch-and-bound and several branch-and-price algorithms for the exact solution of the problem, and improve their performance by the use of lower bounds and tailored optimization techniques. In addition we also develop algorithms for the optimal solution of the related knapsack problem with fragile objects. We conduct an extensive computational evaluation on the benchmark set of instances, and show that the proposed algorithms perform very well.

6.6. Freight railcar routing

In some countries, the activities of managing railroads and managing a fleet of freight railcars are separated by a law. A state-owned company is in charge of the first activity. The control of freight railcars is separated between several independent companies. The main objective of such company is an effective management of its railcars. As these companies are commercial, the goal is to maximize the profit from the usage of their railcars. The profit of a company is mainly determined by the difference between the total gain it receives from satisfying requests for delivery of goods in railcars and the costs it pays to the state-owned company for exploiting the railroad network.

Consequently, the main optimization problem that every freight railcar management company faces can be formulated as follows. We need 1) to choose a set of transportation demands between stations in a railroad network, and 2) to fulfill these demands by appropriately routing the set of available railcars, while maximizing the total profit. We formulate this problem as a multi-commodity flow problem in a large space-time graph. Three approaches are proposed to solve the Linear Programming relaxation of this formulation: direct solution by an LP solver, a column generation approach based on the path reformulation, and a “column generation for

extended formulations" approach [22]. In the latter, the multi-commodity flow formulation is solved iteratively by dynamic generation of arc flow variables. Three approaches have been tested on a set of real-life instances provided by one of the largest freight rail transportation companies in Russia. Instances with up to 10 millions of arc flow variables were solved within minutes of computational time [29], [39].

6.7. Reliable Service Allocation in Clouds with Memory and Capacity Constraints

In [25] we consider allocation problems that arise in the context of service allocation in Clouds. More specifically, on the one part we assume that each Physical Machine (denoted as PM) is offering resources (memory, CPU, disk, network). On the other part, we assume that each application in the IaaS Cloud comes as a set of services running as Virtual Machines (VMs) on top of the set of PMs. In turn, each service requires a given quantity of each resource on each machine where it runs (memory footprint, CPU, disk, network). Moreover, there exists a Service Level Agreement (SLA) between the Cloud provider and the client that can be expressed as follows: the client requires a minimal number of service instances which must be alive at the end of the day, with a given reliability (that can be converted into penalties paid by the provider). In this context, the goal for the Cloud provider is to find an allocation of VMs onto PMs so as to satisfy, at minimal cost, both capacity and reliability constraints for each service. In this paper, we propose a simple model for reliability constraints and we prove that it is possible to derive efficient heuristics.

6.8. On the Theta number of powers of cycle graphs

In [17] we give a closed formula for Lovász's theta number of the powers of cycle graphs C_k^d and of their complements, the circular complete graphs $K_{k/d}$. As a consequence, we establish that the circular chromatic number of a circular perfect graph is computable in polynomial time. We also derive an asymptotic estimate for the theta number of C_k^d.

6.9. Strong chromatic index of planar graphs with large girth

Let Δ be an integer. In [18], we prove that every planar graph with maximum degree Δ and girth at least $10\Delta + 46$ is strong $(2\Delta - 1)$-edge-colorable, that is best possible (in terms of number of colors) as soon as G contains two adjacent vertices of degree Δ. This improves the best previous result when $\Delta \geq 6$.

6.10. Computing clique and chromatic number of circular-perfect graphs in polynomial time

A main result of combinatorial optimization is that clique and chromatic number of a perfect graph are computable in polynomial time (Grötschel et al. in Combinatorica 1(2):169–197,1981). Perfect graphs have the key property that clique and chromatic number coincide for all induced subgraphs; in [19] we address the question whether the algorithmic results for perfect graphs can be extended to graph classes where the chromatic number of all members is bounded by the clique number plus one. We consider a well-studied superclass of perfect graphs satisfying this property, the circular-perfect graphs, and show that for such graphs both clique and chromatic number are computable in polynomial time as well. In addition, we discuss the polynomial time computability of further graph parameters for certain subclasses of circular-perfect graphs. All the results strongly rely upon Lovász's Theta function.

6.11. Computing the clique number of a-perfect graphs in polynomial time

A main result of combinatorial optimization is that clique and chromatic number of a perfect graph are computable in polynomial time (Grötschel, Lovasz and Schrijver 1981). This result relies on polyhedral characterizations of perfect graphs involving the stable set polytope of the graph, a linear relaxation defined by clique constraints, and a semi-definite relaxation, the Theta-body of the graph. A natural question is whether the algorithmic results for perfect graphs can be extended to graph classes with similar polyhedral properties.

In [20] we consider a superclass of perfect graphs, the a-perfect graphs, whose stable set polytope is given by constraints associated with generalized cliques. We show that for such graphs the clique number can be computed in polynomial time as well. The result strongly relies upon Fulkersons's antiblocking theory for polyhedra and Lovasz's Theta function.

SELECT Project-Team

6. New Results

6.1. Model selection in Regression and Classification

Participants: Gilles Celeux, Serge Cohen, Jairo Cugliari, Tim Van Erwen, Clément Levrard, Erwan Le Pennec, Pascal Massart, Nelo Molter Magalhaes, Lucie Montuelle, Mohammed Sedki.

Erwan Le Pennec is still working with Serge Cohen (IPANEMA Soleil) on hyperspectral image segmentation based on a spatialized Gaussian Mixture Model. Their scheme is supported by some theoretical investigation and have been applied in pratice with an efficient minimization algorithm combining EM algorithm, dynamic programming and model selection implemented with MIXMOD. Lucie Montuelle is studying extensions of this model that comprise parametric logistic weights and regression mixtures.

Unsupervised segmentation is an issue similar to unsupervised classification with an added spatial aspect. Functional data is acquired on points in a spatial domain and the goal is to segment the domain in homogeneous domain. The range of applications includes hyperspectral images in conservation sciences, fMRi data and all spatialized functional data. Erwan Le Pennec and Lucie Montuelle are focusing on the questions of the way to handle the spatial component from both the theoretical and the practical point of views. They study in particular the choice of the number of clusters. Furthermore, as functional data require heavy computation, they are required to propose numerically efficient algorithms. They have also extend the model to regression mixture.

Lucie Montuelle focused on conditional density estimation by Gaussian mixtures with logistic weights. Using maximum likelihood estimators, a model selection procedure has been applied, supported by a theoretical guarantee. Numerical experiments have been conducted for regression mixtures with parametric logistic weights, using EM and Newton algorithms. This work is available in the research report and a submitted article.

In collaboration with Lucien Birgé (Université Paris 6), Pascal Massart and Nelo Molter Magalhaes define for the algorithm selection problem a new general cross validation procedure based on robust tests, which is an extension of the hold-out defined by Birgé. They get an original procedure based on the Hellinger distance. This procedure is the unique procedure which does not use any contrast function since it does not estimate the risk. They provide theoretical results showing that, under some weak assumptions on the considered statistical methods, the selected estimator satisfies an oracle type inequality. And, they prove that their robust method can be implemented with a sub-quadratic complexity. Simulations show that their estimator performs generally well for estimating a density with different sample sizes and can handle well-known problems, such as histogram or bandwidth selection.

In collaboration with Gérard Biau (Université Paris 6), Clément Levrard and Pascal Massart provide intuitive conditions have been derived for the k-means clustering algorithm to achieve its optimal rate of convergence. They can be thought of as margin conditions such as ones introduced by Mammen and Tsybakov in the statistical learning framework. These conditions can be checked in many cases, such as Gaussian mixtures with a known number of components and do not require the underlying distribution to have a density, on the contrary to the previous fast rates conditions introduced in this domain. Moreover, It allows to derive non-asymptotic bounds on the mean squared distortion of the k-mean estimator, emphasizing the role played by several other parameters of the quantization issue, such as the smallest distance between optimal codepoints or the excess risk of local minimizers. The influence of these parameters is still in discussion, but some previous results show that some of them are crucial for the minimax results obtained in quantization theory.

Tim van Erven is studying model selection for the long term. When a model selection procedure forms an integrated part of a company's day-to-day activities, its performance should be measured not on a single day, but on average over a longer period, like for example a year. Taking this long-term perspective, it is possible to aggregate model predictions optimally even when the data probability distribution is so irregular that no statistical guarantees can be given for any individual day separately. He studies the relation between model selection for individual days and for the long term, and how the geometry of the models affects both. This work has potential applications in model aggregation for the forecasting of electrical load consumption at EDF. Together with Jairo Cugliari it has also been applied to improve regional forecasts of electrical load consumption using the fact that the consumption of all regions together must add up to the total consumption over the whole country.

The well-documented and consistent variable selection procedure in model-based cluster analysis and classification, that Cathy Maugis (INSA Toulouse) has designed during her PhD. thesis in SELECT, makes use of stepwise algorithms which are painfully slow in high dimensions. In order to circumvent this drawback, Gilles Celeux and Mohammed Sedki, in collaboration with Cathy Maugis, proposed to sort the variables using a lasso-like penalization adapted to the Gaussian mixture model context. Using this rank to select the variables they avoid the combinatory problem of stepwise procedures. Their algorithm is now tested on several challenging simulated and real data sets, showing encouraging performances.

In collaboration with Jean-Michel Marin (Université de Montpellier) and Olivier Gascuel (LIRMM), Gilles Celeux has started a research aiming to select a short list of models rather a single model. This short list of models is declared to be compatible with the data using a p-value derived from the Kullback-Leibler distance between the model and the empirical distribution. And, the Kullback-Leibler distances at hand are estimated trough parametric bootstrap procedures.

6.2. Statistical learning methodology and theory

Participants: Vincent Brault, Gilles Celeux, Christine Keribin, Erwan Le Pennec, Lucie Montuelle, Mesrob Ohannessian, Michel Prenat, Solenne Thivin.

Gilles Celeux, Christine Keribin and the Ph D. student Vincent Brault continued their study on the Latent Block Model (LBM), and worked more especially on categorical data. They further investigated a Gibbs algorithm to avoid solutions with empty clusters on synthetic as well as real data (Congressional Voting Records and genomic data) [STCO13].They detailed the link between the information criteria ICL and BIC, compared them on synthetic and real data, and conjectured that these criteria are both consistent for LBM, which is not a standard behavior. ICL has been proved to be preferred for LBM.

V. Brault applied the Large Gaps algorithm and compared it with other existing algorithms [Aussois13]. He also derived a CEM algorithm for categorical LBM [Agroselect13]. In partnership with the Inria- MODAL team, he implemented the algorithms and information criteria in the R package blockcluster.

C. Keribin has started a collaboration with Tristan Mary-Huard (AgroParisTech) by the supervision of an internship (Master 2) on the use of LBM with truncated Poisson data.

Erwan Le Pennec is supervising Solenne Thivin in her CIFRE with Michel Prenat and Thales Optronique. The aim is target detection on complex background such as clouds or sea. Their approach is a local approach based on test decision theory. They have obtained theoretical and numerical results on a segmentation based approach in which a simple Markov field testing procedure is used in each cell of a data driven partition.

Erwan Le Pennec and Michel Prenat have also collaborated on a cloud texture modeling using a non-parametric approach. Such a modeling coud be used to better calibrate the detection procedure: it can lead to more examples than the one acquired and it could be the basis of an ensemble method.

Mesrob Ohannessian joined SELECT through an ERCIM Alain Bensoussan fellowship. During his stay, his work focused on two different aspects of statistics: large datasets and data scarcity. In collaboration with researchers in ETH Zurich (Prof. Andreas Krause), he studied the possibility of trading off statistical performance and computational speed in the context of k-means clustering, using the notion of coresets. In

collaboration with researchers in Paris 11 (Prof. Elisabeth Gassiat) and Paris 7 (Prof. Stéphane Boucheron), he worked on adaptive universal compression when the alphabet is very large, meaning that some symbol observations are scarce.

6.3. Reliability

Participants: Yves Auffray, Gilles Celeux, Rémy Fouchereau, Patrick Pamphile.

Since 2011, in the framework of a CIFRE convention with Snecma-SAFRAN Rémy Fouchereau has started a thesis on the modeling of fatigue lifetime supervised by Gilles Celeux and Patrick Pamphile. In aircraft, space and nuclear industry, fatigue test is the main basic tool for analyzing fatigue lifetime of a given material, component, or structure. A sample of the material is subjected to cyclic loading S (stress, force, strain, etc.), by a testing machine which counts N, the number of cycles to failure. Fatigue test results are plotted on a SN-curve. A probabilistic model for the construction of SN-curve is proposed. In general, fatigue test results are widely scattered for High Cycle Fatigue region and "duplex" SN-curves appears for Very High Cycle region. That is why classic models from mechanic of rupture theory on one hand, probability theory on the other hand, do not fit SN-curve on the whole range of cycles. We have proposed a probabilistic model, based on a fracture mechanic approach: few parameters are required and they are easily interpreted by mechanic or material engineers.This model has been applied to both simulated and real fatigue test data sets. The SN-curves have been well fitted on the whole range of cycles. The parameters have been estimated using the EM algorithm, combining Newton-Raphson optimisation method and Monte Carlo integral estimations. Recently, the model has been improved taking into account production process information, thanks to a clustering approach. Thus, we have provided engineers with a probabilistic tool for reliability design of mechanical parts, but also with a diagnostic tool for material elaboration.

Since 2013, Gilles Celeux and Patrick Pamphile supervise, in the framework of a collaboration with CEA not yet finalized, a thesis on the modeling of battery State Of Charge for electrical vehicles. Electrical battery is an electrochemical device that converts stored chemical energy into electrical energy. This conversion is reversible and can be repeated during charge/discharge cycles. In an electric vehicle, the battery State Of Charge (SOC) gives the driver indication of how long he can drive without recharging the battery. Unfortunately the complex nature of electrochemical reactions does not allow to measure the SOC directly. Different methods of estimation exist, but they are not robust to various environment conditions (temperature, vehicle driving,...) and to the battery ageing. We propose to estimate the SOC from an *Markov-switching model* : the measurement equation specifies how the SOC depends of an unobservable Markov chain and physical data (temperature, voltage and current intensity,...). Moreover, the SOC estimation is included in the Battery Management System, and therefore estimations must be done online, i.e. with minimum information.

A collaboration has started in 2013 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 penalization tools are intended to be tested on this model selection problem.

6.4. Statistical analysis of genomic data

Participants: Vincent Brault, Gilles Celeux, Christine Keribin.

In collaboration with Florence Jaffrezic and Andrea Rau (INRA, animal genetic department), Mélina Gallopin has started a thesis under the supervision of Gilles Celeux. This thesis is concerned with building statistical networks of genes in animal grenetic. In animal genetic, datasets have a large number of genes and low number of statistical units. For this reason, standard network inference techniques work poorly in this case. At first, this team has developed a data-based method to filter replicated RNA-seq experiments. The method, implemented in the Bioconductor R package `HTSFilter`, removes low expressed genes by optimizing the Jaccard index and reduce the dimension of the dataset. Now, they are studying a clustering model on their expression

profiles measured by RNAseq data using Poisson mixture models. External biological knowledge, such as Gene Ontology annotations are taken into account in the model selection step, based on a approximation of the completed log-likelihood given the annotations.

In collaboration with Marie-Laure Martin-Magniette (URGV), GIlles Celeux and Christine Keribin has started a research concerning the buliding statistical networks of transcription factors (TF) with Gaussian Graphical Models (GGM) in the frawork of the intership of Yann Vasseur (Université Paris-sud) who is starting a PhD. thesis on the same subject at the end of 2013. Since the number of TF is greater than the number of statistical units, a lasso-like procedure is used. Moreover the edges of the network are interpreted using the Latent Block Model studied by Vincent Brault in his thesis. An open issue to be solved is the choice of the regularization parameter in the lasso procedure. It is also important to develop this statistical inference for data with good biological control and knowledge to assess the biological relevance of the proposed models.

6.5. Curves classification, denoising and forecasting

Participants: Jairo Cugliari, Émilie Devijver, Pascal Massart, Jean-Michel Poggi, Vincent Thouvenot.

In collaboration with Farouk Mhamdi and Meriem Jaidane (ENIT, Tunis, Tunisia), Jean-Michel Poggi proposed a method for trend extraction from seasonal time series through the Empirical Mode Decomposition (EMD). Experimental comparison of trend extraction based on EMD, X11, X12 and Hodrick Prescott filter are conducted. First results show the eligibility of the blind EMD trend extraction method. Tunisian real peak load is also used to illustrate the extraction of the intrinsic trend.

Jean-Michel Poggi was the supervisor (with A. Antoniadis) of the PhD Thesis of Jairo Cugliari-Duhalde which takes place in a CIFRE convention with EDF. It was strongly related to the use of wavelets together with curves clustering in order to perform accurate load consumption forecasting. The thesis contains methodological and applied aspects linked to the electrical context as well as theoretical ones by introducing external variables in the context of nonparametric forecasting time series. See http://hal.archives-ouvertes.fr/docs/00/78/82/49/PDF/cugliari-jma.pdf and http://hal.inria.fr/docs/00/55/99/39/PDF/RR-7515.pdf The industrial post-doc of Jairo Cugliari, funded by EDF, explores three aspects of this model that complement the original methodology: first, the construction of a confidence interval for the predictor function, second, the flexibility and simplicity of the model to provide, without extra effort, forecasts horizons further and further away and finally, and third: study of the ability to provide good predictions in the presence of subtle signal nonstationarities induced by loss of customers coming from various scenarios, see http://hal.archives-ouvertes.fr/docs/00/81/49/24/PDF/kwf-suite.pdf

Jean-Michel Poggi, co-supervising with Anestis Antoniadis (Université Joseph Fourier Grenoble) the PhD thesis of Vincent Thouvenot, funded by a CIFRE with EDF. The industrial motivation of this work is the recent development of new technologies for measuring power consumption by EDF to acquire consumption data for different mesh network. The thesis will focus on the development of new statistical methods for predicting power consumption by exploiting the different levels of aggregation of network data collection. From the mathematical point of view, the work is to develop generalized additive models for this type of kind of aggregated data for the modeling of functional data, associating closely nonparametric estimation and variable selection using various penalization methods.

Jean-Michel Poggi and Pascal Massart are the co-advisors of the PhD thesis of Émilie Devijver, strongly motivated by the same kind of industrial forecasting problems in electricity, is dedicated to curves clustering for the prediction. A natural framework to explore this question is mixture of regression models for functional data. The theoretical subject of the thesis is to extend to functional data the recent work by Bühlmann et al. dealing with the simultaneous estimation of mixture regression models in the scalar case using Lasso type methods. Of course, it will be based on the technical tools of the work of Caroline Meynet (which completes her thesis Orsay under the direction of P. Massart), which deals with the clustering of functional data using Lasso methods choosing simultaneously number of clusters and selecting significant wavelet coefficients.

6.6. Neuroimaging, Statistical analysis of fMRI data

Participants: Gilles Celeux, Christine Keribin.

This research takes place as part of a collaboration with Neurospin on brain functional Magnetic Resonance Imaging (fMRI) data. (http://www.math.u-psud.fr/select/reunions/neurospin/Welcome.html). and concerns essentially regularisation in a supervised clustering methodology that includes spatial information in the prediction framework, and yields clustered weighted maps. C. Keribin examined the PhD defence of Virgile Fritsch High-dimensional statistical methods for inter-subjects studies in neuroimaging (Inria, Parietal team).

SequeL Project-Team

6. New Results

6.1. Decision-making Under Uncertainty

6.1.1. Reinforcement Learning

Minimax PAC bounds on the sample complexity of reinforcement learning with a generative model [2]

We consider the problem of learning the optimal action-value function in discounted-reward Markov decision processes (MDPs). We prove new PAC bounds on the sample-complexity of two well-known model-based reinforcement learning (RL) algorithms in the presence of a generative model of the MDP: value iteration and policy iteration. The first result indicates that for an MDP with N state-action pairs and the discount factor γin[0, 1) only O(N log(N/δ)/ [(1 - γ)3 ϵ2]) state-transition samples are required to find an ϵ-optimal estimation of the action-value function with the probability (w.p.) 1-δ. Further, we prove that, for small values of ϵ, an order of O(N log(N/δ)/ [(1 - γ)3 ϵ2]) samples is required to find an ϵ-optimal policy w.p. 1-δ. We also prove a matching lower bound of Ω(N log(N/δ)/ [(1 - γ)3 ϵ2]) on the sample complexity of estimating the optimal action-value function. To the best of our knowledge, this is the first minimax result on the sample complexity of RL: The upper bound matches the lower bound interms of N , ϵ, δ and 1/(1 -γ) up to a constant factor. Also, both our lower bound and upper bound improve on the state-of-the-art in terms of their dependence on 1/(1-γ).

Regret Bounds for Reinforcement Learning with Policy Advice [13]

In some reinforcement learning problems an agent may be provided with a set of input policies, perhaps learned from prior experience or provided by advisors. We present a reinforcement learning with policy advice (RLPA) algorithm which leverages this input set and learns to use the best policy in the set for the reinforcement learning task at hand. We prove that RLPA has a sub-linear regret of $\tilde{O}(\sqrt{T})$ relative to the best input policy, and that both this regret and its computational complexity are independent of the size of the state and action space. Our empirical simulations support our theoretical analysis. This suggests RLPA may offer significant advantages in large domains where some prior good policies are provided.

Optimistic planning for belief-augmented Markov decision processes [11]

This paper presents the Bayesian Optimistic Planning (BOP) algorithm, a novel model-based Bayesian reinforcement learning approach. BOP extends the planning approach of the Optimistic Planning for Markov Decision Processes (OP-MDP) algorithm [10], [9] to contexts where the transition model of the MDP is initially unknown and progressively learned through interactions within the environment. The knowledge about the unknown MDP is represented with a probability distribution over all possible transition models using Dirichlet distributions, and the BOP algorithm plans in the belief-augmented state space constructed by concatenating the original state vector with the current posterior distribution over transition models. We show that BOP becomes Bayesian optimal when the budget parameter increases to infinity. Preliminary empirical validations show promising performance.

Aggregating optimistic planning trees for solving markov decision processes [16]

This paper addresses the problem of online planning in Markov decision processes using a generative model and under a budget constraint. We propose a new algorithm, ASOP, which is based on the construction of a forest of single successor state planning trees, where each tree corresponds to a random realization of the stochastic environment. The trees are explored using a "safe" optimistic planning strategy which combines the optimistic principle (in order to explore the most promising part of the search space first) and a safety principle (which guarantees a certain amount of uniform exploration). In the decision-making step of the algorithm, the individual trees are aggregated and an immediate action is recommended. We provide a finite-sample analysis and discuss the trade-off between the principles of optimism and safety. We report numerical results on a benchmark problem showing that ASOP performs as well as state-of-the-art optimistic planning algorithms.

Optimal Regret Bounds for Selecting the State Representation in Reinforcement Learning [20]

We consider an agent interacting with an environment in a single stream of actions, observations, and rewards, with no reset. This process is not assumed to be a Markov Decision Process (MDP). Rather, the agent has several representations (mapping histories of past interactions to a discrete state space) of the environment with unknown dynamics, only some of which result in an MDP. The goal is to minimize the average regret criterion against an agent who knows an MDP representation giving the highest optimal reward, and acts optimally in it. Recent regret bounds for this setting are of order $O(T^{2/3})$ with an additive term constant yet exponential in some characteristics of the optimal MDP. We propose an algorithm whose regret after T time steps is $O(\sqrt{T})$, with all constants reasonably small. This is optimal in T since $O(\sqrt{T})$ is the optimal regret in the setting of learning in a (single discrete) MDP.

Competing with an Infinite Set of Models in Reinforcement Learning [21]

We consider a reinforcement learning setting where the learner also has to deal with the problem of finding a suitable state-representation function from a given set of models. This has to be done while interacting with the environment in an online fashion (no resets), and the goal is to have small regret with respect to any Markov model in the set. For this setting, recently the BLBãlgorithm has been proposed, which achieves regret of order $T^{2/3}$, provided that the given set of models is finite. Our first contribution is to extend this result to a countably infinite set of models. Moreover, the BLBr˜egret bound suffers from an additive term that can be exponential in the diameter of the MDP involved, since the diameter has to be guessed. The algorithm we propose avoids guessing the diameter, thus improving the regret bound.

A review of optimistic planning in Markov decision processes [30]

We review a class of online planning algorithms for deterministic and stochastic optimal control problems, modeled as Markov decision processes. At each discrete time step, these algorithms maximize the predicted value of planning policies from the current state, and apply the first action of the best policy found. An overall receding-horizon algorithm results, which can also be seen as a type of model-predictive control. The space of planning policies is explored optimistically, focusing on areas with largest upper bounds on the value - or upper confidence bounds, in the stochastic case. The resulting optimistic planning framework integrates several types of optimism previously used in planning, optimization, and reinforcement learning, in order to obtain several intuitive algorithms with good performance guarantees. We describe in detail three recent such algorithms, outline the theoretical guarantees on their performance, and illustrate their behavior in a numerical example.

6.1.2. Multi-arm Bandit Theory

Automatic motor task selection via a bandit algorithm for a brain-controlled button [4]

Objective. Brain-computer interfaces (BCIs) based on sensorimotor rhythms use a variety of motor tasks, such as imagining moving the right or left hand, the feet or the tongue. Finding the tasks that yield best performance, specifically to each user, is a time-consuming preliminary phase to a BCI experiment. This study presents a new adaptive procedure to automatically select (online) the most promising motor task for an asynchronous brain-controlled button. Approach. We develop for this purpose an adaptive algorithm UCB-classif based on the stochastic bandit theory and design an EEG experiment to test our method. We compare (offline) the adaptive algorithm to a naïve selection strategy which uses uniformly distributed samples from each task. We also run the adaptive algorithm online to fully validate the approach. Main results. By not wasting time on inefficient tasks, and focusing on the most promising ones, this algorithm results in a faster task selection and a more efficient use of the BCI training session. More precisely, the offline analysis reveals that the use of this algorithm can reduce the time needed to select the most appropriate task by almost half without loss in precision, or alternatively, allow us to investigate twice the number of tasks within a similar time span. Online tests confirm that the method leads to an optimal task selection. Significance. This study is the first one to optimize the task selection phase by an adaptive procedure. By increasing the number of tasks that can be tested in a given time span, the proposed method could contribute to reducing 'BCI illiteracy'.

Kullback-Leibler Upper Confidence Bounds for Optimal Sequential Allocation [3]

We consider optimal sequential allocation in the context of the so-called stochastic multi-armed bandit model. We describe a generic index policy, in the sense of Gittins (1979), based on upper confidence bounds of the arm payoffs computed using the Kullback-Leibler divergence. We consider two classes of distributions for which instances of this general idea are analyzed: The kl-UCB algorithm is designed for one-parameter exponential families and the empirical KL-UCB algorithm for bounded and finitely supported distributions. Our main contribution is a unified finite-time analysis of the regret of these algorithms that asymptotically matches the lower bounds of Lai and Robbins (1985) and Burnetas and Katehakis (1996), respectively. We also investigate the behavior of these algorithms when used with general bounded rewards, showing in particular that they provide significant improvements over the state-of-the-art.

Sequential Transfer in Multi-armed Bandit with Finite Set of Models [14]

Learning from prior tasks and transferring that experience to improve future performance is critical for building lifelong learning agents. Although results in supervised and reinforcement learning show that transfer may significantly improve the learning performance, most of the literature on transfer is focused on batch learning tasks. In this paper we study the problem of *sequential transfer in online learning*, notably in the multi–armed bandit framework, where the objective is to minimize the total regret over a sequence of tasks by transferring knowledge from prior tasks. Under the assumption that the tasks are drawn from a stationary distribution over a finite set of models, we define a novel bandit algorithm based on a method-of-moments approach for the estimation of the possible tasks and derive regret bounds for it. We introduce a novel bandit algorithm based on a method-of-moments approach for estimating the possible tasks and derive regret bounds for it. Finally, we report preliminary empirical results confirming the theoretical findings.

Optimizing P300-speller sequences by RIP-ping groups apart [25]

So far P300-speller design has put very little emphasis on the design of optimized flash patterns, a surprising fact given the importance of the sequence of flashes on the selection outcome. Previous work in this domain has consisted in studying consecutive flashes, to prevent the same letter or its neighbors from flashing consecutively. To this effect, the flashing letters form more random groups than the original row-column sequences for the P300 paradigm, but the groups remain fixed across repetitions. This has several important consequences, among which a lack of discrepancy between the scores of the different letters. The new approach proposed in this paper accumulates evidence for individual elements, and optimizes the sequences by relaxing the constraint that letters should belong to fixed groups across repetitions. The method is inspired by the theory of Restricted Isometry Property matrices in Compressed Sensing, and it can be applied to any display grid size, and for any target flash frequency. This leads to P300 sequences which are shown here to perform significantly better than the state of the art, in simulations and online tests.

Stochastic Simultaneous Optimistic Optimization [26]

We study the problem of global maximization of a function f given a finite number of evaluations perturbed by noise. We consider a very weak assumption on the function, namely that it is locally smooth (in some precise sense) with respect to some semi-metric, around one of its global maxima. Compared to previous works on bandits in general spaces (Kleinberg et al., 2008; Bubeck et al., 2011a) our algorithm does not require the knowledge of this semi-metric. Our algorithm, StoSOO, follows an optimistic strategy to iteratively construct upper confidence bounds over the hierarchical partitions of the function domain to decide which point to sample next. A finite-time analysis of StoSOO shows that it performs almost as well as the best specifically-tuned algorithms even though the local smoothness of the function is not known.

Toward optimal stratification for stratified monte-carlo integration [9]

We consider the problem of adaptive stratified sampling for Monte Carlo integration of a noisy function, given a finite budget n of noisy evaluations to the function. We tackle in this paper the problem of adapting to the function at the same time the number of samples into each stratum and the partition itself. More precisely, it is interesting to refine the partition of the domain in area where the noise to the function, or where the variations

of the function, are very heterogeneous. On the other hand, having a (too) refined stratification is not optimal. Indeed, the more refined the stratification, the more difficult it is to adjust the allocation of the samples to the stratification, i.e. sample more points where the noise or variations of the function are larger. We provide in this paper an algorithm that selects online, among a large class of partitions, the partition that provides the optimal trade-off, and allocates the samples almost optimally on this partition

Thompson sampling for one-dimensional exponential family bandits [18]

Thompson Sampling has been demonstrated in many complex bandit models, however the theoretical guarantees available for the parametric multi-armed bandit are still limited to the Bernoulli case. Here we extend them by proving asymptotic optimality of the algorithm using the Jeffreys prior for 1-dimensional exponential family bandits. Our proof builds on previous work, but also makes extensive use of closed forms for Kullback-Leibler divergence and Fisher information (and thus Jeffreys prior) available in an exponential family. This allow us to give a finite time exponential concentration inequality for posterior distributions on exponential families that may be of interest in its own right. Moreover our analysis covers some distributions for which no optimistic algorithm has yet been proposed, including heavy-tailed exponential families.

Finite-Time Analysis of Kernelised Contextual Bandits [27]

We tackle the problem of online reward maximisation over a large finite set of actions described by their contexts. We focus on the case when the number of actions is too big to sample all of them even once. However we assume that we have access to the similarities between actions' contexts and that the expected reward is an arbitrary linear function of the contexts' images in the related reproducing kernel Hilbert space (RKHS). We propose KernelUCB, a kernelised UCB algorithm, and give a cumulative regret bound through a frequentist analysis. For contextual bandits, the related algorithm GP-UCB turns out to be a special case of our algorithm, and our finite-time analysis improves the regret bound of GP-UCB for the agnostic case, both in the terms of the kernel-dependent quantity and the RKHS norm of the reward function. Moreover, for the linear kernel, our regret bound matches the lower bound for contextual linear bandits.

From Bandits to Monte-Carlo Tree Search: The Optimistic Principle Applied to Optimization and Planning [33]

This work covers several aspects of the optimism in the face of uncertainty principle applied to large scale optimization problems under finite numerical budget. The initial motivation for the research reported here originated from the empirical success of the so-called Monte-Carlo Tree Search method popularized in computer-go and further extended to many other games as well as optimization and planning problems. Our objective is to contribute to the development of theoretical foundations of the field by characterizing the complexity of the underlying optimization problems and designing efficient algorithms with performance guarantees. The main idea presented here is that it is possible to decompose a complex decision making problem (such as an optimization problem in a large search space) into a sequence of elementary decisions, where each decision of the sequence is solved using a (stochastic) multi-armed bandit (simple mathematical model for decision making in stochastic environments). This so-called hierarchical bandit approach (where the reward observed by a bandit in the hierarchy is itself the return of another bandit at a deeper level) possesses the nice feature of starting the exploration by a quasi-uniform sampling of the space and then focusing progressively on the most promising area, at different scales, according to the evaluations observed so far, and eventually performing a local search around the global optima of the function. The performance of the method is assessed in terms of the optimality of the returned solution as a function of the number of function evaluations. Our main contribution to the field of function optimization is a class of hierarchical optimistic algorithms designed for general search spaces (such as metric spaces, trees, graphs, Euclidean spaces, ...) with different algorithmic instantiations depending on whether the evaluations are noisy or noiseless and whether some measure of the "smoothness" of the function is known or unknown. The performance of the algorithms depend on the local behavior of the function around its global optima expressed in terms of the quantity of near-optimal states measured with some metric. If this local smoothness of the function is known then one can design very efficient optimization algorithms (with convergence rate independent of the space dimension),

and when it is not known, we can build adaptive techniques that can, in some cases, perform almost as well as when it is known.

6.2. Statistical analysis of time series

6.2.1. Change Point Analysis

Nonparametric multiple change point estimation in highly dependent time series [17]

Given a heterogeneous time-series sample, it is required to find the points in time (called change points) where the probability distribution generating the data has changed. The data is assumed to have been generated by arbitrary, unknown, stationary ergodic distributions. No modeling, independence or mixing are made. A novel, computationally efficient, nonparametric method is proposed, and is shown to be asymptotically consistent in this general framework; the theoretical results are complemented with experimental evaluations.

6.2.2. Clustering Time Series, Online and Offline

A Binary-Classification-Based Metric between Time-Series Distributions and Its Use in Statistical and Learning Problems [6]

A metric between time-series distributions is proposed that can be evaluated using binary classification methods, which were originally developed to work on i.i.d. data. It is shown how this metric can be used for solving statistical problems that are seemingly unrelated to classification and concern highly dependent time series. Specifically, the problems of time-series clustering, homogeneity testing and the three-sample problem are addressed. Universal consistency of the resulting algorithms is proven under most general assumptions. The theoretical results are illustrated with experiments on synthetic and real-world data.

6.2.3. Semi-Supervised and Unsupervised Learning

Learning from a Single Labeled Face and a Stream of Unlabeled Data [19]

Face recognition from a single image per person is a challenging problem because the training sample is extremely small. We consider a variation of this problem. In our problem, we recognize only one person, and there are no labeled data for any other person. This setting naturally arises in authentication on personal computers and mobile devices, and poses additional challenges because it lacks negative examples. We formalize our problem as one-class classification, and propose and analyze an algorithm that learns a non-parametric model of the face from a single labeled image and a stream of unlabeled data. In many domains, for instance when a person interacts with a computer with a camera, unlabeled data are abundant and easy to utilize. This is the first paper that investigates how these data can help in learning better models in the single-image-per-person setting. Our method is evaluated on a dataset of 43 people and we show that these people can be recognized 90% of time at nearly zero false positives. This recall is 25+% higher than the recall of our best performing baseline. Finally, we conduct a comprehensive sensitivity analysis of our algorithm and provide a guideline for setting its parameters in practice.

Unsupervised model-free representation learning [23]

Numerous control and learning problems face the situation where sequences of high-dimensional highly dependent data are available, but no or little feedback is provided to the learner. In such situations it may be useful to find a concise representation of the input signal, that would preserve as much as possible of the relevant information. In this work we are interested in the problems where the relevant information is in the time-series dependence. Thus, the problem can be formalized as follows. Given a series of observations $X\_0, \cdots, X\_n$ coming from a large (high-dimensional) space $\mathcal{X}$, find a representation function f mapping $\mathcal{X}$ to a finite space $\mathcal{Y}$ such that the series $f(X\_0), \cdots, f(X\_n)$ preserve as much information as possible about the original time-series dependence in $X\_0, \cdots, X\_n$. For stationary time series, the function f can be selected as the one maximizing the time-series information $I\_\infty(f) = h\_0(f(X)) - h\_\infty(f(X))$ where $h\_0(f(X))$ is the Shannon entropy of $f(X\_0)$ and $h\_\infty(f(X))$ is the entropy rate of the time series

$f(X\_0), \cdots, f(X\_n), \cdots$. In this paper we study the functional $I\_\infty(f)$ from the learning-theoretic point of view. Specifically, we provide some uniform approximation results, and study the behaviour of $I\_\infty(f)$ in the problem of optimal control.

Time-series information and learning [22]

Given a time series $X\_1, \cdots, X\_n, \cdots$ taking values in a large (high-dimensional) space $\mathcal{X}$, we would like to find a function f from $\mathcal{X}$ to a small (low-dimensional or finite) space $\mathcal{Y}$ such that the time series $f(X\_1), \cdots, f(X\_n), \cdots$ retains all the information about the time-series dependence in the original sequence, or as much as possible thereof. This goal is formalized in this work, and it is shown that the target function f can be found as the one that maximizes a certain quantity that can be expressed in terms of entropies of the series $(f(X\_i))\_i \in \mathcal{N}$. This quantity can be estimated empirically, and does not involve estimating the distribution on the original time series $(X\_i)\_i \in \mathcal{N}$.

6.3. Statistical Learning and Bayesian Analysis

6.3.1. Dictionary learning

Learning a common dictionary over a sensor network [10]

We consider the problem of distributed dictionary learning, where a set of nodes is required to collectively learn a common dictionary from noisy measurements. This approach may be useful in several contexts including sensor networks. Diffusion cooperation schemes have been proposed to solve the distributed linear regression problem. In this work we focus on a diffusion-based adaptive dictionary learning strategy: each node records independent observations and cooperates with its neighbors by sharing its local dictionary. The resulting algorithm corresponds to a distributed alternate optimization. Beyond dictionary learning, this strategy could be adapted to many matrix factorization problems in various settings. We illustrate its efficiency on some numerical experiments.

Distributed dictionary learning over a sensor network [29]

We consider the problem of distributed dictionary learning, where a set of nodes is required to collec- tively learn a common dictionary from noisy measure- ments. This approach may be useful in several con- texts including sensor networks. Diffusion cooperation schemes have been proposed to solve the distributed linear regression problem. In this work we focus on a diffusion-based adaptive dictionary learning strategy: each node records observations and cooperates with its neighbors by sharing its local dictionary. The resulting algorithm corresponds to a distributed block coordi- nate descent (alternate optimization). Beyond dictio- nary learning, this strategy could be adapted to many matrix factorization problems and generalized to var- ious settings. This article presents our approach and illustrates its efficiency on some numerical examples.

6.4. Applications

6.4.1. Medical Applications

Outlier detection for patient monitoring and alerting [5]

We develop and evaluate a data-driven approach for detecting unusual (anomalous) patient-management decisions using past patient cases stored in electronic health records (EHRs). Our hypothesis is that a patient-management decision that is unusual with respect to past patient care may be due to an error and that it is worthwhile to generate an alert if such a decision is encountered. We evaluate this hypothesis using data obtained from EHRs of 4486 post-cardiac surgical patients and a subset of 222 alerts generated from the data. We base the evaluation on the opinions of a panel of experts. The results of the study support our hypothesis that the outlier-based alerting can lead to promising true alert rates. We observed true alert rates that ranged from 25% to 66% for a variety of patient-management actions, with 66% corresponding to the strongest outliers.

6.5. Miscellaneous

6.5.1. Miscellaneous

A confidence-set approach to signal denoising [7]

The problem of filtering of finite-alphabet stationary ergodic time series is considered. A method for constructing a confidence set for the (unknown) signal is proposed, such that the resulting set has the following properties. First, it includes the unknown signal with probability γ, where γ is a parameter supplied to the filter. Second, the size of the confidence sets grows exponentially with a rate that is asymptotically equal to the conditional entropy of the signal given the data. Moreover, it is shown that this rate is optimal. We also show that the described construction of the confidence set can be applied to the case where the signal is corrupted by an erasure channel with unknown statistics.

Quantification adaptative pour la stéganalyse d'images texturées [28]

Nous cherchons à améliorer les performances d'un schéma de stéganalyse (i.e. la détection de messages cachées) pour des images texturées. Le schéma de stéganographie étudié consiste à modifier certains pixels de l'image par une perturbation +/-1, et le schéma de stéganalyse utilise les caractéristiques construites à partir de la probabilité conditionnelle empirique de différences de 4 pixels voisins. Dans sa version originale, la stéganalyse n'est pas trés efficace sur des images texturées et ce travail vise àâ€ explorer plusieurs techniques de quantification en utilisant d'abord un pas de quantification plus important puis une quantification adaptative scalaire ou vectorielle. Les cellules de la quantification adaptative sont générées en utilisant un K-means ou un K-means "équilibré" de manière à ce chaque cellule quantifie approximativement le même nombre d'échantillon. Nous obtenons un gain maximal de classification de 3% pour un pas de quantification uniforme de 3. En utilisant l'algorithme K-means équilibré sur [-18,18], le gain par rapport à la version de base est de 4.7%.

Cost-sensitive Multiclass Classification Risk Bounds [8]

A commonly used approach to multiclass classification is to replace the 0-1 loss with a convex surrogate so as to make empirical risk minimization computationally tractable. Previous work has uncovered sufficient and necessary conditions for the consistency of the resulting procedures. In this paper, we strengthen these results by showing how the 0-1 excess loss of a predictor can be upper bounded as a function of the excess loss of the predictor measured using the convex surrogate. The bound is developed for the case of cost-sensitive multiclass classification and a convex surrogate loss that goes back to the work of Lee, Lin and Wahba. The bounds are as easy to calculate as in binary classification. Furthermore, we also show that our analysis extends to the analysis of the recently introduced "Simplex Coding" scheme.

Approximate Dynamic Programming Finally Performs Well in the Game of Tetris [12]

Tetris is a video game that has been widely used as a benchmark for various optimization techniques including approximate dynamic programming (ADP) algorithms. A look at the literature of this game shows that while ADP algorithms that have been (almost) entirely based on approximating the value function (value function based) have performed poorly in Tetris, the methods that search directly in the space of policies by learning the policy parameters using an optimization black box, such as the cross entropy (CE) method, have achieved the best reported results. This makes us conjecture that Tetris is a game in which good policies are easier to represent, and thus, learn than their corresponding value functions. So, in order to obtain a good performance with ADP, we should use ADP algorithms that search in a policy space, instead of the more traditional ones that search in a value function space. In this paper, we put our conjecture to test by applying such an ADP algorithm, called classification-based modified policy iteration (CBMPI), to the game of Tetris. Our experimental results show that for the first time an ADP algorithm, namely CBMPI, obtains the best results reported in the literature for Tetris in both small 10×10 and large 10×20 boards. Although the CBMPI's results are similar to those of the CE method in the large board, CBMPI uses considerably fewer (almost 1/6) samples (calls to the generative model) than CE.

A Generalized Kernel Approach to Structured Output Learning [15]

We study the problem of structured output learning from a regression perspective. We first provide a general formulation of the kernel dependency estimation (KDE) problem using operator-valued kernels. We show that some of the existing formulations of this problem are special cases of our framework. We then propose a covariance-based operator-valued kernel that allows us to take into account the structure of the kernel feature space. This kernel operates on the output space and encodes the interactions between the outputs without any reference to the input space. To address this issue, we introduce a variant of our KDE method based on the conditional covariance operator that in addition to the correlation between the outputs takes into account the effects of the input variables. Finally, we evaluate the performance of our KDE approach using both covariance and conditional covariance kernels on two structured output problems, and compare it to the state-of-the-art kernel-based structured output regression methods.

Gossip-based distributed stochastic bandit algorithms [24]

The multi-armed bandit problem has attracted remarkable attention in the machine learning community and many efficient algorithms have been proposed to handle the so-called exploitation-exploration dilemma in various bandit setups. At the same time, significantly less effort has been devoted to adapting bandit algorithms to particular architectures, such as sensor networks, multi-core machines, or peer-to-peer (P2P) environments, which could potentially speed up their convergence. Our goal is to adapt stochastic bandit algorithms to P2P networks. In our setup, the same set of arms is available in each peer. In every iteration each peer can pull one arm independently of the other peers, and then some limited communication is possible with a few random other peers. As our main result, we show that our adaptation achieves a linear speedup in terms of the number of peers participating in the network. More precisely, we show that the probability of playing a suboptimal arm at a peer in iteration t=Ω(logN) is proportional to 1/(Nt) where N denotes the number of peers. The theoretical results are supported by simulation experiments showing that our algorithm scales gracefully with the size of network.

Sur quelques problèmes non-supervisés impliquant des séries temporelles hautement dèpendantes [1]

Cette thèse est consacrée à l'analyse théorique de problèmes non supervisés impliquant des séries temporelles hautement dépendantes. Plus particulièrement, nous abordons les deux problèmes fondamentaux que sont le problème d'estimation des points de rupture et le partitionnement de séries temporelles. Ces problèmes sont abordés dans un cadre extrêmement général oùles données sont générées par des processus stochastiques ergodiques stationnaires. Il s'agit de l'une des hypothèses les plus faibles en statistiques, comprenant non seulement, les hypothèses de modèles et les hypothèses paramétriques habituelles dans la littérature scientifique, mais aussi des hypothèses classiques d'indépendance, de contraintes sur l'espace mémoire ou encore des hypothèses de mélange. En particulier, aucune restriction n'est faite sur la forme ou la nature des dépendances, de telles sortes que les échantillons peuvent être arbitrairement dépendants. Pour chaque problème abordé, nous proposons de nouvelles méthodes non paramétriques et nous prouvons de plus qu'elles sont, dans ce cadre, asymptotiquement consistantes. Pour l'estimation de points de rupture, la consistance asymptotique se rapporte à la capacité de l'algorithme à produire des estimations des points de rupture qui sont asymptotiquement arbitrairement proches des vrais points de rupture. D'autre part, un algorithme de partitionnement est asymptotiquement consistant si le partitionnement qu'il produit, restreint à chaque lot de séquences, coïncides, à partir d'un certain temps et de manière consistante, avec le partitionnement cible. Nous montrons que les algorithmes proposés sont implémentables efficacement, et nous accompagnons nos résultats théoriques par des évaluations expérimentales. L'analyse statistique dans le cadre stationnaire ergodique est extrêmement difficile. De manière générale, il est prouvé que les vitesses de convergence sont impossibles à obtenir. Dès lors, pour deux échantillons générés indépendamment par des processus ergodiques stationnaires, il est prouvé qu'il est impossible de distinguer le cas où les échantillons sont générés par le même processus de celui où ils sont générés par des processus différents. Ceci implique que des problèmes tels le partitionnement de séries temporelles sans la connaissance du nombre de partitions ou du nombre de points de rupture ne peut admettre de solutions consistantes. En conséquence, une tâche difficile est de découvrir les formulations du problème qui en permettent une résolution dans ce cadre général. La principale contribution de cette thèse est de démon-

trer (par construction) que malgré ces résultats d'impossibilités théoriques, des formulations naturelles des problèmes considérés existent et admettent des solutions consistantes dans ce cadre général. Ceci inclut la démonstration du fait que le nombre de points de rupture corrects peut être trouvé, sans recourir à des hypothèses plus fortes sur les processus stochastiques. Il en résulte que, dans cette formulation, le problème des points de rupture peut être réduit à du partitionnement de séries temporelles. Les résultats présentés dans ce travail formulent les fondations théoriques pour l'analyse des données séquentielles dans un espace d'applications bien plus large.

Actor-Critic Algorithms for Risk-Sensitive MDPs [32]

In many sequential decision-making problems we may want to manage risk by minimizing some measure of variability in rewards in addition to maximizing a standard criterion. Variance-related risk measures are among the most common risk-sensitive criteria in finance and operations research. However, optimizing many such criteria is known to be a hard problem. In this paper, we consider both discounted and average reward Markov decision processes. For each formulation, we first define a measure of variability for a policy, which in turn gives us a set of risk-sensitive criteria to optimize. For each of these criteria, we derive a formula for computing its gradient. We then devise actor-critic algorithms for estimating the gradient and updating the policy parameters in the ascent direction. We establish the convergence of our algorithms to locally risk-sensitive optimal policies. Finally, we demonstrate the usefulness of our algorithms in a traffic signal control application.

Bayesian Policy Gradient and Actor-Critic Algorithms [31]

Policy gradient methods are reinforcement learning algorithms that adapt a parameterized policy by following a performance gradient estimate. Many conventional policy gradient methods use Monte-Carlo techniques to estimate this gradient. The policy is improved by adjusting the parameters in the direction of the gradient estimate. Since Monte-Carlo methods tend to have high variance, a large number of samples is required to attain accurate estimates, resulting in slow convergence. In this paper, we first propose a Bayesian framework for policy gradient, based on modeling the policy gradient as a Gaussian process. This reduces the number of samples needed to obtain accurate gradient estimates. Moreover, estimates of the natural gradient as well as a measure of the uncertainty in the gradient estimates, namely, the gradient covariance, are provided at little extra cost. Since the proposed Bayesian framework considers system trajectories as its basic observable unit, it does not require the dynamic within each trajectory to be of any special form, and thus, can be easily extended to partially observable problems. On the downside, it cannot take advantage of the Markov property when the system is Markovian. To address this issue, we then extend our Bayesian policy gradient framework to actor-critic algorithms and present a new actor-critic learning model in which a Bayesian class of non-parametric critics, based on Gaussian process temporal difference learning, is used. Such critics model the action-value function as a Gaussian process, allowing Bayes' rule to be used in computing the posterior distribution over action-value functions, conditioned on the observed data. Appropriate choices of the policy parameterization and of the prior covariance (kernel) between action-values allow us to obtain closed-form expressions for the posterior distribution of the gradient of the expected return with respect to the policy parameters. We perform detailed experimental comparisons of the proposed Bayesian policy gradient and actor-critic algorithms with classic Monte-Carlo based policy gradient methods, as well as with each other, on a number of reinforcement learning problems.

SIERRA Project-Team

6. New Results

6.1. Block-Coordinate Frank-Wolfe Optimization for Structural SVMs

Participants: Simon Lacoste-Julien [correspondent], Mark Schmidt.

Collaboration with: Martin Jaggi (Centre de Mathématiques Appliquées, Ecole Polytechnique), Patrick Pletscher (Machine Learning Laboratory, ETH Zurich).

In [16] we propose a randomized block-coordinate variant of the classic Frank-Wolfe algorithm for convex optimization with block-separable constraints. Despite its lower iteration cost, we show that it achieves a similar convergence rate in duality gap as the full Frank-Wolfe algorithm. We also show that, when applied to the dual structural support vector machine (SVM) objective, it yields an online algorithm that has the same low iteration complexity as primal stochastic subgradient methods. However, unlike stochastic subgradient methods, the block-coordinate Frank-Wolfe algorithm allows us to compute the optimal step-size and yields a computable duality gap guarantee. Our experiments indicate that this simple algorithm outperforms competing structural SVM solvers.

6.2. Minimizing Finite Sums with the Stochastic Average Gradient.

Participants: Mark Schmidt [correspondent], Nicolas Le Roux, Francis Bach.

In [32] we propose the stochastic average gradient (SAG) method for optimizing the sum of a finite number of smooth convex functions. Like stochastic gradient (SG) methods, the SAG method's iteration cost is independent of the number of terms in the sum. However, by incorporating a memory of previous gradient values the SAG method achieves a faster convergence rate than black-box SG methods. The convergence rate is improved from $O(1/\sqrt{k})$ to $O(1/k)$ in general, and when the sum is strongly-convex the convergence rate is improved from the sub-linear $O(1/k)$ to a linear convergence rate of the form $O(\rho^k)$ for $\rho < 1$. Further, in many cases the convergence rate of the new method is also faster than black-box deterministic gradient methods, in terms of the number of gradient evaluations. Numerical experiments indicate that the new algorithm often dramatically outperforms existing SG and deterministic gradient methods.

The primary contribution of this work is the analysis of a new algorithm that we call the *stochastic average gradient* (SAG) method, a randomized variant of the incremental aggregated gradient (IAG) method of [43]. The SAG method has the low iteration cost of SG methods, but achieves the convergence rates stated above for the FG method. The SAG iterations take the form

$$x^{k+1} = x^k - \frac{\alpha_k}{n} \sum_{i=1}^{n} y_i^k, \tag{20}$$

where at each iteration a random index i_k is selected and we set $y_i^k = f_i'(x^k)$ if $i = i_k$, and y_i^{k-1} otherwise. That is, like the FG method, the step incorporates a gradient with respect to each function. But, like the SG method, each iteration only computes the gradient with respect to a single example and the cost of the iterations is independent of n. Despite the low cost of the SAG iterations, we show in this paper that with a constant step-size *the SAG iterations have an $O(1/k)$ convergence rate for convex objectives and a linear convergence rate for strongly-convex objectives*, like the FG method. That is, by having access to i_k and by keeping a *memory* of the most recent gradient value computed for each index i, this iteration achieves a faster convergence rate than is possible for standard SG methods. Further, in terms of effective passes through the data, we will also see that for many problems the convergence rate of the SAG method is also faster than is possible for standard FG methods.

6.3. Fast Convergence of Stochastic Gradient Descent under a Strong Growth Condition

Participants: Mark Schmidt [correspondent], Nicolas Le Roux [correspondent].

In [33] we consider optimizing a function smooth convex function f that is the average of a set of differentiable functions f_i, under the assumption considered by [87] and [90] that the norm of each gradient f_i' is bounded by a linear function of the norm of the average gradient f'. We show that under these assumptions the basic stochastic gradient method with a sufficiently-small constant step-size has an $O(1/k)$ convergence rate, and has a linear convergence rate if g is strongly-convex.

We write our problem

$$\min_{x \in \mathbb{R}^P} f(x) := \frac{1}{N} \sum_{i=1}^{N} f_i(x), \tag{21}$$

where we assume that f is convex and its gradient f' is Lipschitz-continuous with constant L, meaning that for all x and y we have

$$||f'(x) - f'(y)|| \leq L||x - y||.$$

If f is twice-differentiable, these assumptions are equivalent to assuming that the eigenvalues of the Hessian $f''(x)$ are bounded between 0 and L for all x.

Deterministic gradient methods for problems of this form use the iteration

$$x_{k+1} = x_k - \alpha_k f'(x_k), \tag{22}$$

for a sequence of step sizes α_k. In contrast, *stochastic gradient* methods use the iteration

$$x_{k+1} = x_k - \alpha_k f_i'(x_k), \tag{23}$$

for an individual data sample i selected uniformly at random from the set $\{1, 2, \cdots, N\}$.

The stochastic gradient method is appealing because the cost of its iterations is *independent of*N. However, in order to guarantee convergence stochastic gradient methods require a decreasing sequence of step sizes $\{\alpha_k\}$ and this leads to a slower convergence rate. In particular, for convex objective functions the stochastic gradient method with a decreasing sequence of step sizes has an expected error on iteration k of $O(1/\sqrt{k})$ [78], meaning that

$$\mathbb{E}[f(x_k)] - f(x^*) = O(1/\sqrt{k}).$$

In contrast, the deterministic gradient method with a *constant* step size has a smaller error of $O(1/k)$ [79]. The situation is more dramatic when f is *strongly* convex, meaning that

$$f(y) \geq f(x) + \langle f'(x), y - x \rangle + \frac{\mu}{2}||y - x||^2, \tag{24}$$

for all x and y and some $\mu > 0$. For twice-differentiable functions, this is equivalent to assuming that the eigenvalues of the Hessian are bounded below by μ. For strongly convex objective functions, the stochastic gradient method with a decreasing sequence of step sizes has an error of $O(1/k)$ [77] while the deterministic method with a constant step size has an *linear* convergence rate. In particular, the deterministic method satisfies

$$f(x_k) - f(x^*) \leq \rho^k [f(x_0) - f(x^*)],$$

for some $\rho < 1$ [71].

We show that if the individual gradients $f_i'(x_k)$ satisfy a certain strong growth condition relative to the full gradient $f'(x_k)$, the stochastic gradient method with a sufficiently small constant step size achieves (in expectation) the convergence rates stated above for the deterministic gradient method.

6.4. Non-strongly-convex smooth stochastic approximation with convergence rate $O(1/n)$

Participants: Eric Moulines, Francis Bach [correspondent].

Large-scale machine learning problems are becoming ubiquitous in many areas of science and engineering. Faced with large amounts of data, practitioners typically prefer algorithms that process each observation only once, or a few times. Stochastic approximation algorithms such as stochastic gradient descent (SGD) and its variants, although introduced more than sixty years ago, still remain the most widely used and studied method in this context. In [8], we consider the stochastic approximation problem where a convex function has to be minimized, given only the knowledge of unbiased estimates of its gradients at certain points, a framework which includes machine learning methods based on the minimization of the empirical risk. We focus on problems without strong convexity, for which all previously known algorithms achieve a convergence rate for function values of $O(1/\sqrt{n})$ after n iterations. We consider and analyze two algorithms that achieve a rate of $O(1/n)$ for classical supervised learning problems. For least-squares regression, we show that *averaged* stochastic gradient descent *with constant step-size* achieves the desired rate. For logistic regression, this is achieved by a simple novel stochastic gradient algorithm that (a) constructs successive local quadratic approximations of the loss functions, while (b) preserving the same running-time complexity as stochastic gradient descent. For these algorithms, we provide a non-asymptotic analysis of the generalization error (in expectation, and also in high probability for least-squares), and run extensive experiments showing that they often outperform existing approaches.

6.5. Streaming Bayesian Inference

Participant: Michael Jordan [correspondent].

Large, streaming data sets are increasingly the norm in science and technology. Simple descriptive statistics can often be readily computed with a constant number of operations for each data point in the streaming setting, without the need to revisit past data or have advance knowledge of future data. But these time and memory restrictions are not generally available for the complex, hierarchical models that practitioners often have in mind when they collect large data sets. Significant progress on scalable learning procedures has been made in recent years. But the underlying models remain simple, and the inferential framework is generally non-Bayesian. The advantages of the Bayesian paradigm (e.g., hierarchical modeling, coherent treatment of uncertainty) currently seem out of reach in the Big Data setting.

An exception to this statement is provided by Hofmann et al. (2010), who have shown that a class of approximation methods known as *variational Bayes* (VB) can be usefully deployed for large-scale data sets. They have applied their approach, referred to as *stochastic variational inference* (SVI), to the domain of topic modeling of document collections, an area with a major need for scalable inference algorithms. VB traditionally uses the variational lower bound on the marginal likelihood as an objective function, and the idea of SVI is to apply a variant of stochastic gradient descent to this objective. Notably, this objective is based on the conceptual existence of a full data set involving D data points (i.e., documents in the topic model setting), for a fixed value of D. Although the stochastic gradient is computed for a single, small subset of data points (documents) at a time, the posterior being targeted is a posterior for D data points. This value of D must be specified in advance and is used by the algorithm at each step. Posteriors for D' data points, for D' not equal to D, are not obtained as part of the analysis.

We view this lack of a link between the number of documents that have been processed thus far and the posterior that is being targeted as undesirable in many settings involving streaming data. In this project we aim at an approximate Bayesian inference algorithm that is scalable like SVI but is also truly a streaming procedure, in that it yields an approximate posterior for each processed collection of D' data points—and not just a pre-specified "final" number of data points D. To that end, we return to the classical perspective of Bayesian updating, where the recursive application of Bayes theorem provides a sequence of posteriors, not a sequence of approximations to a fixed posterior. To this classical recursive perspective we bring the VB framework; our updates need not be exact Bayesian updates but rather may be approximations such as VB.

Although the empirical success of SVI is the main motivation for our work, we are also motivated by recent developments in computer architectures, which permit distributed and asynchronous computations in addition to streaming computations. A streaming VB algorithm naturally lends itself to distributed and asynchronous implementations.

6.6. Convex Relaxations for Permutation Problems

Participants: Fajwel Fogel [correspondent], Rodolphe Jenatton, Francis Bach, Alexandre d'Aspremont.

Seriation seeks to reconstruct a linear order between variables using unsorted similarity information. It has direct applications in archeology and shotgun gene sequencing for example. In [12] we prove the equivalence between the seriation and the combinatorial 2-sum problem (a quadratic minimization problem over permutations) over a class of similarity matrices. The seriation problem can be solved exactly by a spectral algorithm in the noiseless case and we produce a convex relaxation for the 2-sum problem to improve the robustness of solutions in a noisy setting. This relaxation also allows us to impose additional structural constraints on the solution, to solve semi-supervised seriation problems. We performed numerical experiments on archeological data, Markov chains and gene sequences.

6.7. Phase retrieval for imaging problems

Participants: Fajwel Fogel [correspondent], Irène Waldspurger, Alexandre d'Aspremont.

In [29] we study convex relaxation algorithms for phase retrieval on imaging problems. We show that structural assumptions on the signal and the observations, such as sparsity, smoothness or positivity, can be exploited to both speed-up convergence and improve recovery performance. We detail experimental results in molecular imaging problems simulated from PDB data.

Phase retrieval seeks to reconstruct a complex signal, given a number of observations on the *magnitude* of linear measurements, i.e. solve

$$\begin{array}{ll} \text{find} & x \\ \text{such that} & |Ax| = b \end{array}$$

in the variable x, where A and b. This problem has direct applications in X-ray and crystallography imaging, diffraction imaging, Fourier optics or microscopy for example, in problems where physical limitations mean detectors usually capture the intensity of observations but cannot recover their phase. In this project, we focus on problems arising in diffraction imaging, where A is usually a Fourier transform, often composed with one or multiple masks (a technique sometimes called ptychography). The Fourier structure, through the FFT, often considerably speeds up basic linear operations, which allows us to solve large scale convex relaxations on realistically large imaging problems. We also observe that in most of the imaging problems we consider, the Fourier transform is very sparse, with known support (we lose the phase but observe the magnitude of Fourier coefficients), which allows us to considerably reduce the size of our convex phase retrieval relaxations.

6.8. Learning Sparse Penalties for Change-point Detection using Max Margin Interval Regression

Participants: Toby Hocking, Guillem Rigaill, Jean-Philippe Vert, Francis Bach [correspondent].

In segmentation models, the number of change-points is typically chosen using a penalized cost function. In [22] we propose to learn the penalty and its constants in databases of signals with weak change-point annotations. We propose a convex relaxation for the resulting interval regression problem, and solve it using accelerated proximal gradient methods. We show that this method achieves state-of-the-art change-point detection in a database of annotated DNA copy number profiles from neuroblastoma tumors.

6.9. Maximizing submodular functions using probabilistic graphical models

Participants: K. S. Sesh Kumar [correspondent], Francis Bach.

In [34] we consider the problem of maximizing submodular functions; while this problem is known to be NP-hard, several numerically efficient local search techniques with approximation guarantees are available. In this paper, we propose a novel convex relaxation which is based on the relationship between submodular functions, entropies and probabilistic graphical models. In a graphical model, the entropy of the joint distribution decomposes as a sum of marginal entropies of subsets of variables; moreover, for any distribution, the entropy of the closest distribution factorizing in the graphical model provides an bound on the entropy. For directed graphical models, this last property turns out to be a direct consequence of the submodularity of the entropy function, and allows the generalization of graphical-model-based upper bounds to any submodular functions. These upper bounds may then be jointly maximized with respect to a set, while minimized with respect to the graph, leading to a convex variational inference scheme for maximizing submodular functions, based on outer approximations of the marginal polytope and maximum likelihood bounded treewidth structures. By considering graphs of increasing treewidths, we may then explore the trade-off between computational complexity and tightness of the relaxation. We also present extensions to constrained problems and maximizing the difference of submodular functions, which include all possible set functions.

Optimizing submodular functions has been an active area of research with applications in graph-cut-based image segmentation [44], sensor placement [69], or document summarization [70]. A set function F is a function defined on the power set 2^V of a certain set V. It is submodular if and only if for all $A, B \subseteq V$, $F(A) + F(B) \geqslant F(A \cap B) + F(A \cup B)$. Equivalently, these functions also admit the diminishing returns property, i.e., the marginal cost of an element in the context of a smaller set is more than its cost in the context of a larger set. Classical examples of such functions are entropy, mutual information, cut functions, and covering functions—see further examples in [58], [38].

Submodular functions form an interesting class of discrete functions because minimizing a submodular function can be done in polynomial time [58], while maximization, although NP-hard, admits constant factor approximation algorithms [76]. In this paper, our ultimate goal is to provide the first (to the best of our knowledge) generic convex relaxation of submodular function maximization, with a hierarchy of complexities related to known combinatorial hierarchies such as the Sherali-Adams hierarchy [83]. Beyond the graphical model tools that we are going to develop, having convex relaxations may be interesting for several reasons:

(1) they can lead to better solutions, (2) they provide online bounds that may be used within branch-and-bound optimization and (3) they ease the use of such combinatorial optimization problems within structured prediction framework [91].

We make the following contributions:

- For any directed acyclic graph G and a submodular function F, we define a bound $F_G(A)$ and study its properties (monotonicity, tightness), which is specialized to decomposable graphs.
- We propose an algorithm to maximize submodular functions by maximizing the bound $F_G(A)$ with respect to A while minimizing with respect to the graph G, leading to a convex variational method based on outer approximation of the marginal polytope [93] and inner approximation of the hypertree polytope.
- We propose extensions to constrained problems and maximizing the difference of submodular functions, which include all possible set functions.
- We illustrate our results on small-scale experiments.

6.10. Reflection methods for user-friendly submodular optimization

Participants: Stefanie Jegelka, Suvrit Sra, Francis Bach [correspondent].

Recently, it has become evident that submodularity naturally captures widely occurring concepts in machine learning, signal processing and computer vision. Consequently, there is need for efficient optimization procedures for submodular functions, especially for minimization problems. While general submodular minimization is challenging, we propose in [15] a new method that exploits existing decomposability of submodular functions. In contrast to previous approaches, our method is neither approximate, nor impractical, nor does it need any cumbersome parameter tuning. Moreover, it is easy to implement and parallelize. A key component of our method is a formulation of the discrete submodular minimization problem as a continuous best approximation problem that is solved through a sequence of reflections, and its solution can be easily thresholded to obtain an optimal discrete solution. This method solves *both* the continuous and discrete formulations of the problem, and therefore has applications in learning, inference, and reconstruction. In our experiments, we illustrate the benefits of our method on two image segmentation tasks.

6.11. Convex Relaxations for Learning Bounded Treewidth Decomposable Graphs

Participants: K. S. Sesh Kumar [correspondent], Francis Bach.

In [24] we consider the problem of learning the structure of undirected graphical models with bounded treewidth, within the maximum likelihood framework. This is an NP-hard problem and most approaches consider local search techniques. In this paper, we pose it as a combinatorial optimization problem, which is then relaxed to a convex optimization problem that involves searching over the forest and hyperforest polytopes with special structures, independently. A supergradient method is used to solve the dual problem, with a run-time complexity of $O(k^3 n^{k+2} \log n)$ for each iteration, where n is the number of variables and k is a bound on the treewidth. We compare our approach to state-of-the-art methods on synthetic datasets and classical benchmarks, showing the gains of the novel convex approach.

Graphical models provide a versatile set of tools for probabilistic modeling of large collections of interdependent variables. They are defined by graphs that encode the conditional independences among the random variables, together with potential functions or conditional probability distributions that encode the specific local interactions leading to globally well-defined probability distributions [42], [93], [67].

In many domains such as computer vision, natural language processing or bioinformatics, the structure of the graph follows naturally from the constraints of the problem at hand. In other situations, it might be desirable to estimate this structure from a set of observations. It allows (a) a statistical fit of rich probability distributions that can be considered for further use, and (b) discovery of structural relationship between different variables. In the former case, distributions with tractable inference are often desirable, i.e., inference with run-time complexity does not scale exponentially in the number of variables in the model. The simplest constraint to ensure tractability is to impose tree-structured graphs [52]. However, these distributions are not rich enough, and following earlier work [73], [39], [75], [48], [59], [89], we consider models with *treewidth* bounded, not simply by one (i.e., trees), but by a small constant k.

Beyond the possibility of fitting tractable distributions (for which probabilistic inference has linear complexity in the number of variables), learning bounded-treewidth graphical models is key to design approximate inference algorithms for graphs with higher treewidth. Indeed, as shown by [82], [93], [68], approximating general distributions by tractable distributions is a common tool in variational inference. However, in practice, the complexity of variational distributions is often limited to trees (i.e., $k = 1$), since these are the only ones with exact polynomial-time structure learning algorithms. The convex relaxation we designed enables us to augment the applicability of variational inference, by allowing a finer trade-off between run-time complexity and approximation quality.

We make the following contributions:

- We provide a novel convex relaxation for learning bounded-treewidth decomposable graphical models from data in polynomial time. This is achieved by posing the problem as a combinatorial optimization problem, which is relaxed to a convex optimization problem that involves the graphic and hypergraphic matroids.
- We show how a supergradient ascent method may be used to solve the dual optimization problem, using greedy algorithms as inner loops on the two matroids. Each iteration has a run-time complexity of $O(k^3 n^{k+2} \log n)$, where n is the number of variables. We also show how to round the obtained fractional solution.
- We compare our approach to state-of-the-art methods on synthetic datasets and classical benchmarks showing the gains of the novel convex approach.

6.12. Large-Margin Metric Learning for Partitioning Problems

Participants: Rémi Lajugie [correspondent], Sylvain Arlot, Francis Bach.

In [31] we consider unsupervised partitioning problems, such as clustering, image segmentation, video segmentation and other change-point detection problems. We focus on partitioning problems based explicitly or implicitly on the minimization of Euclidean distortions, which include mean-based change-point detection, K-means, spectral clustering and normalized cuts. Our main goal is to learn a Mahalanobis metric for these unsupervised problems, leading to feature weighting and/or selection. This is done in a supervised way by assuming the availability of several potentially partially labelled datasets that share the same metric. We cast the metric learning problem as a large-margin structured prediction problem, with proper definition of regularizers and losses, leading to a convex optimization problem which can be solved efficiently with iterative techniques. We provide experiments where we show how learning the metric may significantly improve the partitioning performance in synthetic examples, bioinformatics, video segmentation and image segmentation problems.

Unsupervised partitioning problems are ubiquitous in machine learning and other data-oriented fields such as computer vision, bioinformatics or signal processing. They include (a) traditional *unsupervised clustering* problems, with the classical K-means algorithm, hierarchical linkage methods [61] and spectral clustering [80], (b) *unsupervised image segmentation* problems where two neighboring pixels are encouraged to be in the same cluster, with mean-shift techniques [51] or normalized cuts [84], and (c) *change-point detection* problems adapted to multivariate sequences (such as video) where segments are composed of contiguous elements, with typical window-based algorithms [54] and various methods looking for a change in the mean of the features (see, e.g., [49]).

All the algorithms mentioned above rely on a specific distance (or more generally a similarity measure) on the space of configurations. A good metric is crucial to the performance of these partitioning algorithms and its choice is heavily problem-dependent. While the choice of such a metric has been originally tackled manually (often by trial and error), recent work has considered learning such metric directly from data. Without any supervision, the problem is ill-posed and methods based on generative models may learn a metric or reduce dimensionality (see, e.g., [53]), but typically with no guarantees that they lead to better partitions. In this paper, we follow [41], [95], [40] and consider the goal of learning a metric for potentially several partitioning problems sharing the same metric, assuming that several fully or partially labelled partitioned datasets are available during the learning phase. While such labelled datasets are typically expensive to produce, there are several scenarios where these datasets have already been built, often for evaluation purposes. These occur in video segmentation tasks, image segmentation tasks as well as change-point detection tasks in bioinformatics (see [62]).

W consider partitioning problems based explicitly or implicitly on the minimization of Euclidean distortions, which include K-means, spectral clustering and normalized cuts, and mean-based change-point detection. We make the following contributions:

- We review and unify several partitioning algorithms, and cast them as the maximization of a linear function of a rescaled equivalence matrix, which can be solved by algorithms based on spectral relaxations or dynamic programming.
- Given fully labelled datasets, we cast the metric learning problem as a large-margin structured prediction problem, with proper definition of regularizers, losses and efficient loss-augmented inference.
- Given partially labelled datasets, we propose an algorithm, iterating between labeling the full datasets given a metric and learning a metric given the fully labelled datasets. We also consider extensions that allow changes in the full distribution of univariate time series (rather than changes only in the mean), with application to bioinformatics.
- We provide experiments where we show how learning the metric may significantly improve the partitioning performance in synthetic examples, video segmentation and image segmentation problems.

6.13. Comparison between multi-task and single-task oracle risks in kernel ridge regression

Participant: Matthieu Solnon [correspondent].

In [35] we study multi-task kernel ridge regression and try to understand when the multi-task procedure performs better than the single-task one, in terms of averaged quadratic risk. In order to do so, we compare the risks of the estimators with perfect calibration, the oracle risk. We are able to give explicit settings, favorable to the multi-task procedure, where the multi-task oracle performs better than the single-task one. In situations where the multi-task procedure is conjectured to perform badly, we also show the oracle does so. We then complete our study with simulated examples, where we can compare both oracle risks in more natural situations. A consequence of our result is that the multi-task ridge estimator has a lower risk than any single-task estimator, in favorable situations.

Increasing the sample size is the most common way to improve the performance of statistical estimators. In some cases (see, for instance, the experiments of [56] on customer data analysis or those of [63] on molecule binding problems), having access to some new data may be impossible, often due to experimental limitations. One way to circumvent those constraints is to use datasets from several related (and, hopefully, “similar”) problems, as if it gave additional (in some sense) observations on the initial problem. The statistical methods using this heuristic are called “multi-task” techniques, as opposed to “single-task” techniques, where every problem is treated one at a time. In this paper, we study kernel ridge regression in a multi-task framework and try to understand when multi-task can improve over single-task.

The first trace of a multi-task estimator can be found in the work of [88]. In this article, Charles Stein showed that the usual maximum-likelihood estimator of the mean of a Gaussian vector (of dimension larger than 3, every dimension representing here a task) is not admissible—that is, there exists another estimator that has a lower risk for every parameter. He showed the existence of an estimator that uniformly attains a lower quadratic risk by shrinking the estimators along the different dimensions towards an arbitrary point. An explicit form of such an estimator was given by [64], yielding the famous James-Stein estimator. This phenomenon, now known as the "Stein's paradox", was widely studied in the following years and the behaviour of this estimator was confirmed by empirical studies, in particular the one from [55]. This first example clearly shows the goals of the multi-task procedure: an advantage is gained by borrowing information from different tasks (here, by shrinking the estimators along the different dimensions towards a common point), the improvement being scored by the global (averaged) squared risk. Therefore, this procedure does not guarantee individual gains on every task, but a global improvement on the sum of those task-wise risks.

We consider $p \geq 2$ different regression tasks, a framework we refer to as "multi-task" regression, and where the performance of the estimators is measured by the fixed-design quadratic risk. Kernel ridge regression is a classical framework to work with and comes with a natural norm, which often has desirable properties (such as, for instance, links with regularity). This norm is also a natural "similarity measure" between the regression functions. [56] showed how to extend kernel ridge regression to a multi-task setting, by adding a regularization term that binds the regression functions along the different tasks together. One of the main questions that is asked is to assert whether the multi-task estimator has a lower risk than any single-task estimator. It was recently proved by [86] that a fully data-driven calibration of this procedure is possible, given some assumptions on the set of matrices used to regularize—which correspond to prior knowledge on the tasks. Under those assumptions, the estimator is showed to verify an *oracle inequality*, that is, its risk matches (up to constants) the best possible one, the *oracle risk*. Thus, it suffices to compare the oracle risks for the multi-task procedure and the single-task one to provide an answer to this question.

We study the oracle multi-task risk and compare it to the oracle single-task risk. We then find situations where the multi-task oracle is proved to have a lower risk than the single-task oracle. This allows us to better understand which situation favors the multi-task procedure and which does not. After having defined our model, we write down the risk of a general multi-task ridge estimator and see that it admits a convenient decomposition using two key elements: the mean of the tasks and the resulting variance. This decomposition allows us to optimize this risk and get a precise estimation of the oracle risk, in settings where the ridge estimator is known to be minimax optimal. We then explore several repartitions of the tasks that give the latter multi-task rates, study their single-task oracle risk and compare it to their respective multi-task rates. This allows us to discriminate several situations, depending whether the multi-task oracle either outperforms its single-task counterpart, underperforms it or whether both behave similarly. We also show that, in the cases favorable to the multi-task oracle detailed in the previous sections, the estimator proposed by [86] behaves accordingly and achieves a lower risk than the single-task oracle. We finally study settings where we can no longer explicitly study the oracle risk, by running simulations, and we show that the multi-task oracle continues to retain the same virtues and disadvantages as before.

6.14. Sharp analysis of low-rank kernel matrix approximations

Participant: Francis Bach [correspondent].

Kernel methods, such as the support vector machine or kernel ridge regression, are now widely used in many areas of science and engineering, such as computer vision or bioinformatics. However, kernel methods typically suffer from at least quadratic running-time complexity in the number of observations n, as this is the complexity of computing the kernel matrix. In large-scale settings where n may be large, this is usually not acceptable. In [7], we consider supervised learning problems within the positive-definite kernel framework, such as kernel ridge regression, kernel logistic regression or the support vector machine. Low-rank approximations of the kernel matrix are often considered as they allow the reduction of running time complexities to $O(p^2 n)$, where p is the rank of the approximation. The practicality of such methods thus depends on the required rank p. In this paper, we show that in the context of kernel ridge regression, for

approximations based on a random subset of columns of the original kernel matrix, the rank p may be chosen to be linear in the *degrees of freedom* associated with the problem, a quantity which is classically used in the statistical analysis of such methods, and is often seen as the implicit number of parameters of non-parametric estimators. This result enables simple algorithms that have sub-quadratic running time complexity, but provably exhibit the same *predictive performance* than existing algorithms, for any given problem instance, and not only for worst-case situations.

6.15. fMRI encoding and decoding models

Participant: Fabian Pedregosa [correspondent].

In [20] we show that HRF estimation improves sensitivity of fMRI encoding and decoding models and propose a new approach for the estimation of Hemodynamic Response Functions from fMRI data. The model we propose is based on the linearity assumption behind the General Linear Model and can be computed using standard gradient-based solvers. We use the activation patterns computed by our model as input data for encoding and decoding studies and report performance improvement in both settings.

This work proves that significant improvements in recovery of brain activation patterns can be made by estimating the form of the Hemodynamic Response Function instead of using a canonical form for this response.

6.16. Structured Penalties for Log-linear Language Models

Participants: Anil Nelakanti [correspondent], Cédric Archambeau, Francis Bach, Guillaume Bouchard.

Language models can be formalized as log-linear regression models where the input features represent previously observed contexts up to a certain length m. The complexity of existing algorithms to learn the parameters by maximum likelihood scale linearly in nd, where n is the length of the training corpus and d is the number of observed features. In [19] we present a model that grows logarithmically in d, making it possible to efficiently leverage longer contexts. We account for the sequential structure of natural language using tree-structured penalized objectives to avoid overfitting and achieve better generalization.

Language models are crucial parts of advanced natural language processing pipelines, such as speech recognition [45], machine translation [47], or information retrieval [92]. When a sequence of symbols is observed, a language model predicts the probability of occurrence of the next symbol in the sequence. Models based on so-called back-off smoothing have shown good predictive power [60]. In particular, Kneser-Ney (KN) and its variants [66] are still achieving state-of-the-art results for more than a decade after they were originally proposed. Smoothing methods are in fact clever heuristics that require tuning parameters in an ad-hoc fashion. Hence, more principled ways of learning language models have been proposed based on maximum entropy [50] or conditional random fields [81], or by adopting a Bayesian approach [94].

We focus on penalized maximum likelihood estimation in log-linear models. In contrast to language models based on *unstructured* norms such as ℓ_2 (quadratic penalties) or ℓ_1 (absolute discounting), we use *tree-structured* norms [96], [65]. Structured penalties have been successfully applied to various NLP tasks, including chunking and named entity recognition [74], but not language modeling. Such penalties are particularly well-suited to this problem as they mimic the nested nature of word contexts. However, existing optimizing techniques are not scalable for large contexts m.

We show that structured tree norms provide an efficient framework for language modeling. Furthermore, we give the first algorithm for structured ℓ_∞ tree norms with a complexity nearly linear in the number of nodes. This leads to a memory-efficient *and* time-efficient learning algorithm for generalized linear language models.

6.17. Distributed Large-scale Natural Graph Factorization

Participants: Amr Ahmed, Nino Shervashidze [correspondent], Shravan Narayanamurthy, Vanja Josifovski, Alexander Smola.

Natural graphs, such as social networks, email graphs, or instant messaging patterns, have become pervasive through the internet. These graphs are massive, often containing hundreds of millions of nodes and billions of edges. While some theoretical models have been proposed to study such graphs, their analysis is still difficult due to the scale and nature of the data. We propose a framework for large-scale graph decomposition and inference. To resolve the scale, our framework in [6] is distributed so that the data are partitioned over a shared-nothing set of machines. We propose a novel factorization technique that relies on partitioning a graph so as to minimize the number of neighboring vertices rather than edges across partitions. Our decomposition is based on a streaming algorithm. It is network-aware as it adapts to the network topology of the underlying computational hardware. We use local copies of the variables and an efficient asynchronous communication protocol to synchronize the replicated values in order to perform most of the computation without having to incur the cost of network communication. On a graph of 200 million vertices and 10 billion edges, derived from an email communication network, our algorithm retains convergence properties while allowing for almost linear scalability in the number of computers.

6.18. Evaluating Speech Features with the Minimal-Pair ABX task

Participants: Thomas Schatz [correspondent], Vijayaditya Peddinti, Francis Bach, Aren Jansen, Hynek Hermansky, Emmanuel Dupoux.

In [23] we introduce a new framework for the evaluation of speech representations in zero-resource settings, that extends and complements previous work by Carlin, Jansen and Hermansky [46]. In particular, we replace their Same/Different discrimination task by several Minimal-Pair ABX (MP-ABX) tasks. We explain the analytical advantages of this new framework and apply it to decompose the standard signal processing pipelines for computing PLP and MFC coefficients. This method enables us to confirm and quantify a variety of well-known and not-so-well-known results in a single framework.

Speech recognition technology crucially rests on adequate speech features for encoding input data. Several such features have been proposed and studied (MFCCs, PLPs, etc), but they are often evaluated indirectly using complex tasks like phone classification or word identification. Such an evaluation technique suffers from several limitations. First, it requires a large enough annotated corpus in order to train the classifier/recognizer. Such a resource may not be available in all languages or dialects (the so-called "zero or limited resource" setting). Second, supervised classifiers may be too powerful and may compensate for potential defects of speech features (for instance noisy/unreliable channels). However, such defects are problematic in unsupervised learning techniques. Finally, the particular statistical assumptions of the classifier (linear, Gaussian, etc.) may not be suited for specific speech features (for instance sparse neural codes as in Hermansky [85]). It is therefore important to replace these complex evaluation schemes by simpler ones which tap more directly the properties of the speech features.

We extend and complement the framework proposed by Carlin, Jansen and Hermansky [46] for the evaluation of speech features in zero resource settings. This framework uses a Same-Different word discrimination task that does not depend on phonetically labelled data, nor on training a classifier. It assumes a speech corpus segmented into words, and derives a word-by-word acoustic distance matrix computed by comparing every word with every other one using Dynamic Time Warping (DTW). Carlin et al. then compute an average precision score which is used to evaluate speech features (the higher average precision, the better the features).

We explore an extension of this technique through Minimal-Pair ABX tasks (MP-ABX tasks) tested on a phonetically balanced corpus [57]. This improves the interpretability of the Carlin et al evaluation results in three different ways. First, the Same/Different task requires the computation of a ROC curve in order to derive average precision. In contrast, the ABX task is a discrimination task used in psychophysics (see [72], chapter 9) which allows for the direct computation of an error rate or a d' measure that are easier to interpret than average precision [46] and involve no assumption about ROC curves. Second, the Same/Different task compares *sets of words*, and as a result is influenced by the mix of similar versus distinct words or short versus long words in the corpus. The ABX task, in contrast, is computed on *word pairs*, and therefore enables to make linguistically precise comparisons, as in word *minimal pairs*, i.e. words differing by only one phoneme. Variants of the task enable to study phoneme discrimination across talkers and/or phonetic contexts, as well as

talker discrimination across phonemes. Because it is more controlled and provides a parameter and model-free metric, the MP-ABX error rate also enables to compare performance across databases or across languages. Third, we compute bootstrap-based estimates of the variability of our performance measures, which allows us to derive confidence intervals for the error rates and tests of the significance of the difference between the error rates obtained with different representations.

6.19. Hidden Markov Tree Models for Semantic Class Induction

Participants: Edouard Grave [correspondent], Guillaume Obozinski, Francis Bach.

In [13] we propose a new method for semantic class induction. First, we introduce a generative model of sentences, based on dependency trees and which takes into account homonymy. Our model can thus be seen as a generalization of Brown clustering. Second, we describe an efficient algorithm to perform inference and learning in this model. Third, we apply our proposed method on two large datasets (10^8 tokens, 10^5 words types), and demonstrate that classes induced by our algorithm improve performance over Brown clustering on the task of semi-supervised supersense tagging and named entity recognition.

Most competitive learning methods for computational linguistics are supervised, and thus require labeled examples, which are expensive to obtain. Moreover, those techniques suffer from data scarcity: many words only appear a small number of time, or even not at all, in the training data. It thus helps a lot to first learn word clusters on a large amount of unlabeled data, which are cheap to obtain, and then to use this clusters as features for the supervised task. This scheme has proven to be effective for various tasks such as named entity recognition, syntactic chunking or syntactic dependency parsing. It was also successfully applied for transfer learning of multilingual structure.

The most commonly used clustering method for semi-supervised learning is known as Brown clustering. While still being one of the most efficient word representation method, Brown clustering has two limitations we want to address in this work. First, since it is a hard clustering method, homonymy is ignored. Second, it does not take into account syntactic relations between words, which seems crucial to induce semantic classes. Our goal is thus to propose a method for semantic class induction which takes into account both syntax and homonymy, and then to study their effects on semantic class learning.

We start by introducing a new unsupervised method for semantic classes induction. This is achieved by defining a generative model of sentences with latent variables, which aims at capturing semantic roles of words. We require our method to be scalable, in order to learn models on large datasets containing tens of millions of sentences. More precisely, we make the following contributions:

- We introduce a generative model of sentences, based on dependency trees, which can be seen as a generalization of Brown clustering,
- We describe a fast approximate inference algorithm, based on message passing and online EM for scaling to large datasets. It allowed us to learn models with 512 latent states on a dataset with hundreds of millions of tokens in less than two days on a single core,
- We learn models on two datasets, Wikipedia articles about musicians and the NYT corpus, and evaluate them on two semi-supervised tasks, namely supersense tagging and named entity recognition.

6.20. Domain Adaptation for Sequence Labeling using Hidden Markov Models

Participants: Edouard Grave [correspondent], Guillaume Obozinski, Francis Bach.

Most natural language processing systems based on machine learning are not robust to domain shift. For example, a state-of-the-art syntactic dependency parser trained on Wall Street Journal sentences has an absolute drop in performance of more than ten points when tested on textual data from the Web. An efficient solution to make these methods more robust to domain shift is to first learn a word representation using large amounts of unlabeled data from both domains, and then use this representation as features in a supervised learning algorithm. In this paper, we propose to use hidden Markov models to learn word representations for part-of-speech tagging. In particular, we study the influence of using data from the source, the target or both domains to learn the representation and the different ways to represent words using an HMM.

Nowadays, most natural language processing systems are based on supervised machine learning. Despite the great successes obtained by those techniques, they unfortunately still suffer from important limitations. One of them is their sensitivity to domain shift: for example, a state-of-the-art part-of-speech tagger trained on the Wall Street Journal section of the Penn treebank achieves an accuracy of 97% when tested on sentences from the Wall Street Journal, but only 90% when tested on textual data from the Web. This drop in performance can also be observed for other tasks such as syntactic parsing or named entity recognition.

One of the explanations for this drop in performance is the big lexical difference that exists accross domains. This results in a lot of out-of-vocabulary words (OOV) in the test data, *i.e.*, words of the test data that were not observed in the training set. For example, more than 25% of the tokens of the test data from the Web corpus are unobserved in the training data from the WSJ. By comparison, only 11.5% of the tokens of the test data from the WSJ are unobserved in the training data from the WSJ. Part-of-speech taggers make most of their errors on those out-of-vocabulary words.

Labeling enough data to obtain a high accuracy for each new domain is not a viable solution. Indeed, it is expensive to label data for natural language processing, because it requires expert knowledge in linguistics. Thus, there is an important need for transfer learning, and more precisely for domain adaptation, in computational linguistics. A common solution consists in using large quantities of unlabeled data, from both source and target domains, in order to learn a good word representation. This representation is then used as features to train a supervised classifier that is more robust to domain shift. Depending on how much data from the source and the target domains are used, this method can be viewed as performing semi-supervised learning or domain adaptation. The goal is to reduce the impact of out-of-vocabulary words on performance. This scheme was first proposed to reduce data sparsity for named entity recognition, before being applied to domain adaptation for part-of-speech tagging or syntactic parsing.

Hidden Markov models have already been considered in previous work to learn word representations for domain adaptation or semi-supervised learning. Our contributions in [25] are mostly experimental: we compare different word representations that can be obtained from an HMM and study the effect of training the unsupervised HMM on source, target or both domains. While previous work mostly use Viterbi decoding to obtain word representations from an HMM, we empirically show that posterior distributions over latent classes give better results.

6.21. Simple Greedy Matching for Aligning Large Knowledge Bases

Participant: Simon Lacoste-Julien [correspondent].

Collaboration with: Konstantina Palla, Alex Davies, Zoubin Ghahramani (Machine Learning Group, Department of Engineering, University of Cambridge), Gjergji Kasneci (Max Planck Institut für Informatik), Thore Graepel (Microsoft Research Cambridge)

The Internet has enabled the creation of a growing number of large-scale knowledge bases in a variety of domains containing complementary information. Tools for automatically aligning these knowledge bases would make it possible to unify many sources of structured knowledge and answer complex queries. However, the efficient alignment of large-scale knowledge bases still poses a considerable challenge. Here, we present Simple Greedy Matching (SiGMa), a simple algorithm for aligning knowledge bases with millions of entities and facts. SiGMa is an iterative propagation algorithm that leverages both the structural information from the relationship graph and flexible similarity measures between entity properties in a greedy local search, which makes it scalable. Despite its greedy nature, our experiments in [17] indicate that SiGMa can efficiently match some of the world's largest knowledge bases with high accuracy. We provide additional experiments on benchmark datasets which demonstrate that SiGMa can outperform state-of-the-art approaches both in accuracy and efficiency.

TAO Project-Team

6. New Results

6.1. Continuous Optimization

Participants: Ouassim Ait Elhara, Yohei Akimoto, Asma Atamna, Anne Auger, Alexandre Chotard, Nikolaus Hansen, Ilya Loshchilov, Yann Ollivier, Marc Schoenauer, Michèle Sebag, Olivier Teytaud.

Our expertise in continuous optimization is focused on stochastic search algorithms. We address theory, algorithm design, and applications. The methods we investigate are adaptive techniques that are able to learn iteratively the parameters of the distribution used to sample (new) solutions. The Covariance Matrix Adaptation Evolution Strategy (CMA-ES) is nowadays one of the most powerful methods for derivative-free continuous optimization. We work on different variants of the CMA-ES to improve it in various contexts as described below. We have previously proven the convergence of simplified variants of the CMA-ES algorithm using the theory of stochastic approximation, and have provided the first proofs of convergence on composite of twice continuously differentiable functions. More recently, we used Markov chain analysis for analyzing the step-size adaptation rules of evolution strategies related to the CMA-ES algorithm.

Surrogate models for CMA-ES. In the context of his PhD thesis defended in January 2013 [4], Ilya Loshchilov has proposed different surrogate variants of CMA-ES based on ranking-SVM that preserve the invariance to monotonic transformation of the CMA-ES algorithm. As a follow-up, he has proposed an original over-exploitation mechanism in case of accurate surrogate [44]. Several of these models have entered the BBOB-2013 workshop [43]. Further research direction using the KL divergence between successive distributions as a trigger for a new learning phase has been proposed [45].

Step-size adaptive methods. We have proposed a new step-size adaptation mechanism that can loosely be interpreted as a new variant of the 1/5 success rule for comma (non-elitist) strategies and which is applicable with a large population size [21]. The rule uses the success of the median fitness of the current population compared to a (different) fitness percentile from the previous population.

Principles of Stochastic Optimization. Based on the framework of *information geometry* (IGO), theoretical guarantees have been obtained for continuous optimization algorithms: using the *natural gradient* provides improvement guarantees even when using finite step sizes [22]. We have considered the principles of designing effective stochastic optimization algorithms from the bottom-up and the top-down perspective [56]. The top-down perspective takes the information-geometrical view-point and largely confirms the bottom-up construction.

Benchmarking. We have continued our effort for improving standards in benchmarking and pursued the development of the COCO (COmparing Continuous Optimizers) platform (see Section 5.4). We have organized the ACM GECCO 2013 workshop on Black-Box-Optimization Benchmarking [2] and benchmarked different surrogate-based variants of the CMA-ES algorithm [26], [44], [43]. Our new starting ANR project NumBBO, centered on the COCO platform, aims at extending it for large-scale, expensive, constrained and multi-objective optimization.

Theoretical proofs of convergence. We have established the connection between convergence of comparison based step-size adaptive randomized search and the stability analysis of some underlying Markov chains. This connection heavily exploits invariance properties of the algorithm. In a first paper we establish this connection for scaling-invariant functions and prove sufficient conditions for linear convergence expressed in terms of stability conditions [63]. We have proven, using this defined methodology, the linear convergence of a famous algorithm introduced independently by several researchers and known as the (1+1)-ES with one-fifth success rule [62]. In [32], we have proven the linear convergence of a modified evolutionary algorithm without assuming quasi-convexity.

[2] see http://coco.gforge.inria.fr/doku.php?id=bbob-2013

6.2. Optimal Decision Making under Uncertainty

Participants: Olivier Teytaud [correspondent], Jean-Joseph Christophe, Adrien Couëtoux, Jérémie Decock, Nicolas Galichet, Manuel Loth, Marc Schoenauer, Michèle Sebag.

The UCT-SIG works on sequential optimization problems, where a decision has to be made at each time step along a finite time horizon, and the underlying problem involves uncertainties along an either adversarial or stochastic setting.

The most prominent application domain is now energy management, at various time scales, and more generally, planning in uncertain environments. The main advances done this year include:

- A work on metagaming/investment [12], where a macroscopic decision has to be made (e.g., investment decisions, which plants should be built) prior to operational decisions (e.g., unit commitment policy, i.e., the operational management of the system). This is a key part of our activity for 2014.
- Bandit problems with risk [36]. Bandit problems are quite related to metagaming problems (they correspond to the unstructured case).
- A theoretical work on the consistency of Monte Carlo Tree Search / Upper Confidence Tree in continuous domains [27]. A non-trivial extension was necessary for proving such a consistency.
- Noisy optimization is a key part of our work [61], as it is crucial for direct policy search or more generally for dynamic optimization:
  - We have proven lower bounds under "locality assumptions" [33], which are usually informally assumed by some practicionners for justifying the use of evolutionary algorithms.
  - In cases with strong noise (variance not decreasing to zero around the optimum) we proved log-log convergence for simple rules for choosing the number of resamplings [23].
- Several submissions are joint works with Ailab, National Dong Hwa University, Hualien, Taiwan. The drafts can be found at http://www.lri.fr/~teytaud/indema.html.
- In collaboration with Christian Shulte (KTH, Stockholm), one of the main contributors to the well-known general-purpose CP solver *GECODE* (http://www.gecode.org/), and within the Microsoft-Inria joint lab Adapt project, ideas from UCT have been integrated in GECODE for the choice of the variable values during the exploration of the constraint tree. The most critical issue lied in the definition of a meaningful reward for a given node (variable = value) that could cope with the multiple restarts of the search: the deeper the failure, the larger the reward (and hence this work also pertains to the CRI-SIG(Section 6.4). Initial results have been obtained with job-shop scheduling problems [47] and more extensive results have been obtained on 3 benchmarks of the CP community [46].

6.3. Distributed Systems

Participants: Cécile Germain-Renaud [correspondent], Philippe Caillou, Dawei Feng, Cyril Furtlehner, Victorin Martin, Michèle Sebag.

The DIS-SIG explores the issues related to modeling and optimizing distributed systems, ranging from very large scale computational grids to multi-agent systems and large scale traffic management.

Fault management. As Lamport formulated decades ago, fault management in distributed systems exemplifies the unreachability of exact prior knowledge. Real-world large scale systems additionally face the non-stationarity issue.

[20] models the system state and its ruptures (non-stationarity) through the flow of jobs as a stream (scalability), with a traceability goal (interpretability), and addresses a key difficulty in Data Streaming, which is timely detection of a change in the generative process underlying the data stream *drift*. A statistical model based on spatial distance and time frequency is proposed, together with adaptive thresholding. Theoretical and experimental validation show the robustness of the method.

D. Feng's PhD formulates the problem of probe selection for fault prediction based on end-to-end probing as a Collaborative Prediction (CP) problem, based on the reasonable assumption of an underlying factorial model [13]. Monitoring large scale distributed systems differ from CP's usual applications (personalized recommendation), in two major ways. On the brighter side, while users cannot be queried for specific recommendations, probes can be launched at will. On the downside, firstly the distribution of the probe results is highly skewed, faults being a small fraction of the total population, and secondly, some of the faults are transient. Amongst the numerous approaches addressing CP, Minimum Margin Matrix Factorization (MMMF) is easily amenable to active learning, which addresses fault sparsity both at spatial (skewed distributions) and temporal (transients) level. From extensive experiments on real-world data, we have shown that modelling probe-based fault prediction as a CP task and addressing this task through MMMF is an extremely efficient strategy for fault prediction. Comparative analysis and experiments motivate the critical advantage of active learning. It offers a scalable alternative to direct AUC optimization. Similarly, comparison with bias-aware methods (Mixed Membership Matrix Factorization) indicates that the capacity of actively selecting the most informative probes provides the most efficient method to capture the time variability of the system.

Multi-agent and games. Resuming earlier work, our goal is to provide an automated abstract description of simulation results. Data mining methods are used to identify groups in complex simulations [11]. Using activity indicators to identify the most interesting agent groups [17], the groups and their evolution are described through one or several simulations [10]. To facilitate the dissemination of the algorithms, we have participated in the development of a generic multiagent platform (GAMA), in collaboration with IRD, University of Rouen (IDEES), and University of Toulouse (IRIT) [34], [35].

A statistical physics perspective. With motivating applications in large scale traffic congestion inference problems, we have

- Settled a method for encoding real data with pairwise dependencies into an Ising copula [58] suitable to infer real-valued data (travel time) from the computation of its corresponding latent binary state (congested/not congested) probabilities.
- In parallel we have investigated the inverse Ising problem, proposing among other methods a loop analysis based on a duality transformation, leading to a dual belief propagation algorithm runing on the dual graph formed by the network of independent cycles. This aims at finding an MRF to represent pairwise correlated data, close to a dependence tree, able to take into account most important loops [14], [15].

6.4. Designing Criteria

Participants: Jamal Atif, Yoann Isaac, Mostepha Redouane Khouadjia, Hélène Paugam-Moisy, Marc Schoenauer, Michèle Sebag.

This recently created SIG, rooted on the claim that *What matters is the criterion*, aims at defining new learning or optimization objectives reflecting fundamental properties of the model, the problem or the expert prior knowledge.

Image understanding. We continued our effort on the development of model-based image understanding approaches (e.g. [71]). In [18], we have proposed a method for simultaneously segmenting and recognizing objects in images, based on a structural representation of the scene and on a constraint propagation method. Theoretical guaranties have been provided along with a quantitative assessment on healthy and pathological brain structures in magnetic resonance images. Within the ANR project LOGIMA (collaboration with ECP, Telecom PariTech and TU Dresden), our goal is to introduce a new lattice-based representation and reasoning framework suited for dealing with spatial objects in the presence of uncertainty. This framework associates under the aegis of general lattice theory ingredients from mathematical morphology, description logics and formal concept analysis. A first development of this framework can be found in [7] where it has been exploited for the definition of

abductive reasoning services and applied to high-level image understanding. Several theoretical issues have been raised in the development of this new framework. Some of them were tackled in [25], [24], [30]. In [25], we have shown how mathematical morphology operators can ben defined on general concept lattices. Explicit join-commuting and meet-commuting operators are defined either from particular valuations on the corresponding lattice or from the decomposition of their elements. In [24], we extended our mathematical morphology based adductive reasoning to multivalued logics, hence allowing us to deal with several uncertainty and imprecision phenomena. In [30], metrics between bipolar information - where the information is represented by a positive/preference part and a negative/constraint part - have been introduced based on particular dilations.

Structured learning. With motivations in bio-informatics and brain computer interfaces, the goal is to take into account priors about the spatio-temporal structure of the underlying phenomenon in order to propose a generative model of the data.

In the context of Yoann Isaac's PhD (Digiteo Unsupervised Brain project), in collaboration with CEA LIST, the goal is to design a representation endowed with appropriate invariance properties. Specifically, within the framework of sparse dictionary coding, we have introduced new priors allowing us to capture both spatial and temporal regularity of multivariate brainwave signals [54]. The learning/optimization criterion, while being multivariate, contains several non-differentiable terms, raising new optimization issues; the proposed approach extends the classical split Bregman iterations algorithm to the multi-dimensional case with several non-differentiable terms [37].

In the context of regulatory gene networks, the challenge is to combine probabilistic inference (does a gene regulate another one) with relational learning (the set of genes is organized in a network). Ensemble learning approaches have been used to cope with the imbalanced nature of the data, e.g., bagging Markov logic networks or boosting operator-valued kernel-based regressors [55], [64]. Another issue, regarding the indeterminacy of the models due to the data sparsity, is addressed through prior-guided regularization beyond model sparsity such as orthogonality [8] or stability [16].

In the domain of medical imaging, the exploitation of computational tomography data to model tumor physiology is hindered by the huge noise level; the multi-task setting is leveraged to provide a better robustness to noise [51].

Robotic value systems. Within the European SYMBRION IP, investigations on the preference-based reinforcement learning were continued in Riad Akrour's PhD, where the robot demonstrations are assessed by the expert and these assessments are used to learn a model of the expert's expectations. In [67], this work had been extended and combined with active learning to yield state-of-the art performances with few binary feedbacks from the expert. The work has first concentrated this year on handling the noise due to expert's mistakes [53], and bridging the reality gap when porting the algorithms on real robots (e-pucks and one Nao robot) – these results will be published in Riad Akrour's PhD dissertation, to be defended in Spring 2014.

Algorithm Selection as Collaborative Filtering. The crucial issue when addressing algorithm selection problems is to be able to come up with features that can describe the problems: with representative features, algorithm selection amounts to supervised learning. However, except for some rare domaines (e.g., SAT, [73]), no satisfying set of features exists. However, algorithm selection can also be viewed as a recommendation problem, and tackled by collaborative filtering: users more or less like movies, and similarly, instances like algorithms as much as these algorithms are efficient in solving it. Applying collaborative filtering leads to designing a latent feature space in which the representation of the problems is highly adapted to the algorithm selection problem. A critical issue in collaborative filtering is the 'cold start' problem, that is making recommendations for a brand new user/problem instance. This issue has been handled by a surrogate model of the latent factors, mapping the initial features onto the latent ones. The *Algorithm Recommender System* has been successfully applied to 3 different domains: Satisfiability, Constraint Programming, and Continuous Black-Box Optimization (data from the COCO platform, see Section 5.4) [59].

Social Networks with insider information. The analysis of social networks based on the contents and

structure of information exchanges most often pertains to descriptive learning, e.g., explaining the growth of the communication graph or investigating the sensitivity of existing algorithms to hyper-parameters [31]. In the Modyrum context (coll. SME Augure), a supervised learning perspective is investigated, taking advantage of the fact that experts already know part of the sought results in some specific domains of interest. Based on e.g., Twitter and blogs data, the goal is to define generic features and supervised learning algorithms, enabling to characterize the targets of interest depending on the public relation focus.

Multi-objective AI Planning. Within the ANR project DESCARWIN (http://descarwin.lri.fr), Mostepha-Redouane Kouadjia continued his work on the **multi-objective approach** to AI Planning using the Evolutionary Planner *Divide-and-Evolve* (DaE), that evolves a sequential decomposition of the problem at hand: each sub-problem is then solved in turn by some embedded classical planner [70]. Even though the embedded planner is single-objective, DaE can nevertheless handle multi-objective problems. Current work includes the implementation of the multi-objective version of DaE, the definition of some benchmark suite, and some first numerical experiments, comparing in particular the results of a full Pareto approach to those of the classical aggregation method. These works resulted in 3 conference papers recently accepted, introducing a tunable benchmark test suite [39], demonstrating that the best quality measure for parameter tuning in this multi-objective framework is the hypervolume, even in the case of the aggregation approach [41], and comparing the evolutionary multi-objective approach with the aggregation method, the only method known to the AI Planning community [38]. A sum-up of these recent results have been published at IJCAI [40].

ALEA Project-Team

6. New Results

6.1. Sparsity-Promoting Bayesian Dynamic Linear Models

Sparsity-promoting priors have become increasingly popular over recent years due to an increased number of regression and classification applications involving a large number of predictors. In time series applications where observations are collected over time, it is often unrealistic to assume that the underlying sparsity pattern is fixed. We propose an original class of flexible Bayesian linear models for dynamic sparsity modelling. The proposed class of models expands upon the existing Bayesian literature on sparse regression using generalized multivariate hyperbolic distributions. The properties of the models are explored through both analytic results and simulation studies. We demonstrate the model on a financial application where it is shown that it accurately represents the patterns seen in the analysis of stock and derivative data, and is able to detect major events by filtering an artificial portfolio of assets.

6.2. Evolutionnary algorithms and genetic programming

The regularity of a signal can be numerically expressed using Hölder exponents, which characterize the singular structures a signal contains. In particular, within the domains of image processing and image understanding, regularity-based analysis can be used to describe local image shape and appearance. However, estimating the Hölder exponent is not a trivial task, and current methods tend to be computationally slow and complex. This work presents an approach to automatically synthesize estimators of the pointwise Hölder exponent for digital images. This task is formulated as an optimization problem and Genetic Programming (GP) is used to search for operators that can approximate a traditional estimator, the oscillations method. Experimental results show that GP can generate estimators that achieve a low error and a high correlation with the ground truth estimation. Furthermore, most of the GP estimators are faster than traditional approaches, in some cases their runtime is orders of magnitude smaller. This result allowed us to implement a real-time estimation of the Hölder exponent on a live video signal, the first such implementation in current literature. Moreover, the evolved estimators are used to generate local descriptors of salient image regions, a task for which a stable and robust matching is achieved, comparable with state-of-the-art methods. In conclusion, the evolved estimators produced by GP could help expand the application domain of Hölder regularity within the fields of image analysis and signal processing.

One of the main open problems within Genetic Programming (GP) is to meaningfully characterize the difficulty (or hardness) of a problem. The general goal is to develop predictive tools that can allow us to identify how difficult a problem is for a GP system to solve. On this topic, we identify and compare two main approaches that address this question. We denote the first group of methods as Evolvability Indicators (EI), which are measures that attempt to capture how amendable the fitness landscape is to a GP search. The best examples of current EIs are the Fitness Distance Correlation (FDC) and the Negative Slope Coefficient (NSC). The second, more recent, group of methods are what we call Predictors of Expected Performance (PEP), which are predictive models that take as input a set of descriptive attributes of a particular problem and produce as output the expected performance of a GP system. The experimental work presented here compares an EI, the NSC, and a PEP model for a GP system applied to data classification. Results suggest that the EI fails at measuring problem difficulty expressed by the performance of the GP classifiers, an unexpected result. On the other hand, the PEP models show a very high correlation with the actual performance of the GP system. It appears that while an EI can correctly estimate the difficulty of a given search, as shown by previous research on this topic, it does not necessarily capture the difficulty of the underlying problem that GP is intended to solve. Conversely, while the PEP models treat the GP system as a computational black-box, they can still provide accurate performance predictions.

Another research area is to predict the alertness of an individual by analyzing the brain activity through electroencephalographic data (EEG) captured with 58 electrodes. Alertness is characterized here as a binary variable that can be in a "normal" or "relaxed" state. We collected data from 44 subjects before and after a relaxation practice, giving a total of 88 records. After a pre-processing step and data validation, we analyzed each record and discriminate the alertness states using our proposed "slope criterion". Afterwards, several common methods for supervised classification (k nearest neighbors, decision trees (CART), random forests, PLS and discriminant sparse PLS) were applied as predictors for the state of alertness of each subject. The proposed "slope criterion" was further refined using a genetic algorithm to select the most important EEG electrodes in terms of classification accuracy. Results shown that the proposed strategy derives accurate predictive models of alertness.

6.3. Moderate Deviations for Mean Field Particle Models

Our team is interested with moderate deviation principles of a general class of mean field type interacting particle models. We discuss functional moderate deviations of the occupation measures for both the strong - topology on the space of finite and bounded measures as well as for the corresponding stochastic processes on some class of functions equipped with the uniform topology. Our approach is based on an original semigroup analysis combined with stochastic perturbation techniques and projective limit large deviation methods.

6.4. Bifurcating autoregressive processes

We investigate the asymptotic behavior of the least squares estimator of the unknown parameters of random coefficient bifurcating autoregressive processes. Under suitable assumptions on inherited and environmental effects, we establish the almost sure convergence of our estimates. In addition, we also prove a quadratic strong law and central limit theorems. Our approach mainly relies on asymptotic results for vector-valued martingales together with the well-known Rademacher-Menchov theorem.

We study also the asymptotic behavior of the weighted least square estimators of the unknown parameters of random coefficient bifurcating autoregressive processes. Under suitable assumptions on the immigration and the inheritance, we establish the almost sure convergence of our estimators, as well as a quadratic strong law and central limit theorems. Our study mostly relies on limit theorems for vector-valued martingales.

Finally, we study the asymptotic behavior of the weighted least squares estimators of the unknown parameters of bifurcating integer-valued autoregressive processes. Under suitable assumptions on the immigration, we establish the almost sure convergence of our estimators, together with the quadratic strong law and central limit theorems. All our investigation relies on asymptotic results for vector-valued martingales.

6.5. Durbin-Watson statistic and first order autoregressive processes

We investigate moderate deviations for the Durbin-Watson statistic associated with the stable first-order autoregressive process where the driven noise is also given by a first-order autoregressive process. We first establish a moderate deviation principle for both the least squares estimator of the unknown parameter of the autoregressive process as well as for the serial correlation estimator associated with the driven noise. It enables us to provide a moderate deviation principle for the Durbin-Watson statistic in the easy case where the driven noise is normally distributed and in the more general case where the driven noise satisfies a less restrictive Chen-Ledoux type condition.

We investigate the asymptotic behavior of the Durbin-Watson statistic for the general stable $p-$order autoregressive process when the driven noise is given by a first-order autoregressive process. We establish the almost sure convergence and the asymptotic normality for both the least squares estimator of the unknown vector parameter of the autoregressive process as well as for the serial correlation estimator associated with the driven noise. In addition, the almost sure rates of convergence of our estimates are also provided. Then, we prove the almost sure convergence and the asymptotic normality for the Durbin-Watson statistic. Finally, we propose a new bilateral statistical procedure for testing the presence of a significative first-order residual autocorrelation and we also explain how our procedure performs better than the commonly used Box-Pierce and Ljung-Box statistical tests for white noise applied to the stable autoregressive process, even on small-sized samples.

In a recent paper (to appear hal-00677600), we investigate the asymptotic behavior of the maximum Likelihood estimators of the unknown parameters of positive recurrent Ornstein-Uhlenbeck processes driven by Ornstein-Uhlenbeck processes.

6.6. Ornstein-Uhlenbeck process with shift

We investigate the large deviation properties of the maximum likelihood estimators for the Ornstein-Uhlenbeck process with shift. We estimate simultaneously the drift and shift parameters. On the one hand, we establish a large deviation principle for the maximum likelihood estimates of the drift and shift parameters. Surprisingly, we find that the drift estimator shares the same large deviation principle as the one previously established for the Ornstein-Uhlenbeck process without shift. Sharp large deviation principles are also provided. On the other hand, we show that the maximum likelihood estimator of the shift parameter satisfies a large deviation principle with a very unusual implicit rate function.

6.7. Markovian superquadratic BSDEs

In [Stochastc Process. Appl., 122(9):3173-3208], the author proved the existence and the uniqueness of solutions to Markovian superquadratic BSDEs with an unbounded terminal condition when the generator and the terminal condition are locally Lipschitz. In [8], we prove that the existence result remains true for these BSDEs when the regularity assumptions on the generator and/or the terminal condition are weakened.

6.8. Non-Asymptotic Analysis of Adaptive and Annealed Feynman-Kac Particle Models

Sequential and Quantum Monte Carlo methods, as well as genetic type search algorithms can be interpreted as a mean field and interacting particle approximations of Feynman-Kac models in distribution spaces. The performance of these population Monte Carlo algorithms is strongly related to the stability properties of nonlinear Feynman-Kac semigroups. We analyze these models in terms of Dobrushin ergodic coefficients of the reference Markov transitions and the oscillations of the potential functions. Sufficient conditions for uniform concentration inequalities w.r.t. time are expressed explicitly in terms of these two quantities. We provide an original perturbation analysis that applies to annealed and adaptive FK models, yielding what seems to be the first results of this kind for these type of models. Special attention is devoted to the particular case of Boltzmann-Gibbs measures' sampling. In this context, we design an explicit way of tuning the number of Markov Chain Monte Carlo iterations with temperature schedule. We also propose and analyze an alternative interacting particle method based on an adaptive strategy to define the temperature increments.

6.9. A Robbins-Monro procedure for a class of models of deformation

We are interested with the statistical analysis of several data sets associated with shape invariant models with different translation, height and scaling parameters. We propose to estimate these parameters together with the common shape function. Our approach extends the recent work of Bercu and Fraysse to multivariate shape invariant models. We propose a very efficient Robbins-Monro procedure for the estimation of the translation parameters and we use these estimates in order to evaluate scale parameters. The main pattern is estimated by a weighted Nadaraya-Watson estimator. We provide almost sure convergence and asymptotic normality for all estimators. Finally, we illustrate the convergence of our estimation procedure on simulated data as well as on real ECG data.

6.10. Individual load curves intraday forecasting

A dynamic coupled modelling is investigated to take temperature into account in the individual energy consumption forecasting. The objective is both to avoid the inherent complexity of exhaustive SARIMAX models and to take advantage of the usual linear relation between energy consumption and temperature for thermosensitive customers. We first recall some issues related to individual load curves forecasting. Then,

we propose and study the properties of a dynamic coupled modelling taking temperature into account as an exogenous contribution and its application to the intraday prediction of energy consumption. Finally, these theoretical results are illustrated on a real individual load curve. The authors discuss the relevance of such an approach and anticipate that it could form a substantial alternative to the commonly used methods for energy consumption forecasting of individual customers.

ASPI Project-Team

5. New Results

5.1. Iterative isotone regression

Participant: Arnaud Guyader.

This is a collaboration with Nicolas Hengartner (Los Alamos), Nicolas Jégou (université de Rennes 2) and Eric Matzner–Løber (université de Rennes 2), and with Alexander B. Németh (Babeş Bolyai University) and Sándor Z. Németh (University of Birmingham).

We explore some theoretical aspects of a recent nonparametric method for estimating a univariate regression function of bounded variation. The method exploits the Jordan decomposition which states that a function of bounded variation can be decomposed as the sum of a non-decreasing function and a non-increasing function. This suggests combining the backfitting algorithm for estimating additive functions with isotonic regression for estimating monotone functions. The resulting iterative algorithm is called IIR (iterative isotonic regression). The main result in this work [22] states that the estimator is consistent if the number of iterations k_n grows appropriately with the sample size n. The proof requires two auxiliary results that are of interest in and by themselves: firstly, we generalize the well-known consistency property of isotonic regression to the framework of a non-monotone regression function, and secondly, we relate the backfitting algorithm to the von Neumann algorithm in convex analysis. We also analyse how the algorithm can be stopped in practice using a data-splitting procedure.

With the geometrical interpretation linking this iterative method with the von Neumann algorithm, and making a connection with the general property of isotonicity of projection onto convex cones, we derive in [14] another equivalent algorithm and go further in the analysis.

5.2. Mutual nearest neighbors

Participant: Arnaud Guyader.

This is a collaboration with Nicolas Hengartner (Los Alamos).

Motivated by promising experimental results, this work [13] investigates the theoretical properties of a recently proposed nonparametric estimator, called the MNR (mutual nearest neighbors) rule, which estimates the regression function $m(x) = E[Y|X = x]$ as follows: first identify the k nearest neighbors of x in the sample, then keep only those for which x is itself one of the k nearest neighbors, and finally take the average over the corresponding response variables. We prove that this estimator is consistent and that its rate of convergence is optimal. Since the estimate with the optimal rate of convergence depends on the unknown distribution of the observations, we also have adaptation results by data-splitting.

5.3. Adaptive multilevel splitting

Participants: Frédéric Cérou, Arnaud Guyader, Florent Malrieu.

This is a collaboration with Pierre Del Moral (EPI ALEA, Inria Bordeaux—Sud Ouest).

We show that an adaptive version of multilevel splitting for rare events is strongly consistent. We also show that the estimates satisfy a CLT (central limit theorem), with the same asymptotic variance as the non-adaptive algorithm with the optimal choice of the parameters. It is a strong and general result, that generalizes some of our previous results, and the proof is quite technical and involved.

5.4. Total variation estimates for the TCP process

Participant: Florent Malrieu.

This is a collaboration with Jean-Baptiste Bardet (université de Rouen), Alejandra Christen (University of Chile), Arnaud Guillin (université de Clermont–Ferrand), and Pierre–André Zitt (université de Paris–Est Marne–la–Vallée).

The TCP window size process appears in the modeling of the famous Transmission Control Protocol used for data transmission over the Internet. This continuous time Markov process takes its values in $[0, \infty)$, is ergodic and irreversible. The sample paths are piecewise linear deterministic and the whole randomness of the dynamics comes from the jump mechanism. The aim of [27] is to provide quantitative estimates for the exponential convergence to equilibrium, in terms of the total variation and Wasserstein distances, using coupling methods. The technique could be applied to a large class of Markov processes as well.

5.5. On the stability of planar randomly switched systems

Participant: Florent Malrieu.

This is a collaboration with Michel Benaïm (université de Neuchâtel), Stéphane Le Borgne (IRMAR) and Pierre–André Zitt (université de Paris–Est Marne–la–Vallée).

The paper [28] illustrates some surprising instability properties that may occur when stable ODE's are switched using Markov dependent coefficients. Consider the random process (X_t) solution of $dX_t/dt = A(I_t)X_t$ where (I_t) is a Markov process on $\{0, 1\}$ and A_0 and A_1 are real Hurwitz matrices on $\mathbb{R}^2$. Assuming that there exists $\lambda \in (0, 1)$ such that $(1 - \lambda)A_0 + \lambda A_1$ has a positive eigenvalue, we establish that the norm of X_t may converge to 0 or infinity, depending on the the jump rate of the process I. An application to product of random matrices is studied. This work can be viewed as a probabilistic counterpart of the paper [26] by Baldé, Boscain and Mason.

5.6. Marginalization in rare event simulation for switching diffusions

Participant: François Le Gland.

This is a collaboration with Anindya Goswami (IISER, Poone).

Switching diffusions are continuous–time Markov processes with a hybrid continuous / finite state space. A rare but critical event (such as a scalar function of the continuous component of the state exceeding a given threshold) can occur for several reasons:

- the process can remain in *nominal* mode, where the critical event is very unlikely to occur,
- or the process can switch in some *degraded* mode, where the critical event is much more likely to occur, but the switching itself is very unlikely to occur.

Not only is it important to accurately estimate the (very small) probability that the critical event occurs before some fixed final time, but it is also important to have an accurate account on the reason why it occured, or in other words to estimate the probability of the different modes. A classical implementation of the multilevel splitting would not be efficient. Indeed, as soon as (even a few) samples paths switch to a *degraded* mode, these sample paths will dominate and it will not be possible to estimate the contribution of samples paths in the *nominal* mode. Moreover, sampling the finite component of the state is not efficient to accurately estimate the (very small) probability of rare but critical modes. A more efficient implementation is based on marginalization, i.e. in sampling jointly the continuous component and the probability distribution of the finite component given the past continuous component [18]. The latter is a probability vector, known as the Wonham filter, that satisfies a deterministic equation.

5.7. Combining importance sampling and multilevel splitting for rare event simulation

Participants: François Le Gland, Damien–Barthélémy Jacquemart.

This is a collaboration with Jérôme Morio (ONERA, Palaiseau).

The problem is to accurately estimate the (very small) probability that a rare but critical event (such as a scalar function of the state exceeding a given threshold) occurs before some fixed final time. Multilevel splitting is a very efficient solution, in which sample paths are propagated and are replicated when some intermediate events occur. Events that are defined in terms of the state variable only (such as a scalar function of the state exceeding an intermediate threshold) are not a good design. A more efficient but more complicated design would be to let the intermediate events depend also on time. An alternative design is to keep intermediate events simple, defined in terms of the state variable only, and to make sure that samples that exceed the threshold early are replicated more than samples that exceed the same threshold later [19].

5.8. Sequential data assimilation: ensemble Kalman filter vs. particle filter

Participants: François Le Gland, Valérie Monbet.

The contribution has been to prove (by induction) the asymptotic normality of the estimation error, i.e. to prove a central limit theorem for the ensemble Kalman filter. Explicit expression of the asymptotic variance has been obtained for linear Gaussian systems (where the exact solution is known, and where EnKF is unbiased). This expression has been compared with explicit expressions of the asymptotic variance for two popular particle filters: the bootstrap particle filter and the so–called optimal particle filter, that uses the next observation in the importance distribution.

5.9. Non–homogeneous Markov–switching models

Participant: Valérie Monbet.

This is a collaboration with Pierre Ailliot (université de Bretagne occidentale, Brest).

We have developped various hidden non–homogeneous Markov–switching models for description and simulation of univariate and multivariate time series. Considered application are in weather variables modelling but also in economy. The main originality of the proposed models is that the hidden Markov chain is not homogeneous, its evolution depending on the past wind conditions or other covariates. It is shown that it permits to reproduce complex non–linearities.

5.10. Dynamical partitioning of directional ocean wave spectra

Participant: Valérie Monbet.

This is a collaboration with Pierre Ailliot (université de Bretagne occidentale, Brest) and Christophe Maisondieu (IFREMER, Brest).

Directional wave spectra generally exhibit several peaks due to the coexistence of wind sea generated by local wind conditions and swells originating from distant weather systems. The paper [24] proposes a new algorithm for partitioning such spectra and retrieving the various systems which compose a complex sea-state. It is based on a sequential Monte Carlo algorithm which allows to follow the time evolution of the various systems. The proposed methodology is validated on both synthetic and real spectra and the results are compared with a method commonly used in the literature.

5.11. Track–before–detect

Participants: François Le Gland, Alexandre Lepoutre.

This is a collaboration with Olivier Rabaste (ONERA, Palaiseau).

The problem considered in [20] is tracking one or several targets in a track–before–detect (TBD) context using particle filters. These filters require the computation of the likelihood of the complex measurement given the target states. This likelihood depends on the complex amplitudes of the targets. When the complex amplitude fluctuates over time, time coherence of the target cannot be taken into account. However, for the single target case, spatial coherence of this amplitude can be taken into account to improve the filter performance, by marginalizing the likelihood of the complex measurement over the amplitude parameter. The marginalization depends on the fluctuation law considered. We show that for the Swerling 1 model the likelihood of the complex measurement can be obtained analytically in the multi-target case. For the Swerling 0 model no closed form can be obtained in the general multi–target setting. Therefore we resort to some approximations to solve the problem. Finally, we demonstrate with Monte Carlo simulations the gain of this method both in detection and in estimation compared to the classic method that works with the square modulus of the complex signal.

The problem considered in [21] is detecting and tracking a single radar target with amplitude fluctuation Swerling 1 and 3 in a track–before–detect context with particle filter. Those fluctuations are difficult to take into account as they are uncoherent from measurement to measurement. Thus, conventionnal filters work on square modulus of the complexe signal to remove the unknown phase of complex amplitude and the marginalized over the law of the modulus but they lose the spatial coherence of the amplitude in the measurement. We show in this paper that complex measurements can be marginalized directly while taking into account the spatial coherence of the complex amplitude. Finally, we show the benefit of this method both in detection and in estimation via Monte Carlo simulations.

CQFD Project-Team

6. New Results

6.1. Nonparametric estimation of the jump rate for non-homogeneous marked renewal processes.

Participants: Romain Azais, François Dufour, Anne Gégout-Petit.

Non-homogeneous marked renewal process, nonparametric estimation, jump rate estimation, Nelson-Aalen estimator, asymptotic consistency, ergodicity of Markov chains

This work is devoted to the nonparametric estimation of the jump rate and the cumulative rate for a general class of non-homogeneous marked renewal processes, defined on a separable metric space. In our framework, the estimation needs only one observation of the process within a long time. Our approach is based on a generalization of the multiplicative intensity model, introduced by Aalen in the seventies. We provide consistent estimators of these two functions, under some assumptions related to the ergodicity of an embedded chain and the characteristics of the process. A numerical example illustrates our theoretical results.

It has been published in Ann. Inst. H. Poincaré Probab. Statist. [16].

6.2. Nonparametric estimation of the conditional distribution of the inter-jumping times for piecewise-deterministic markov processes

Participants: Romain Azais, François Dufour, Anne Gégout-Petit.

Piecewise-deterministic Markov process, ergodicity of Markov chains, nonparametric estimation, jump rate estimation, Nelson-Aalen estimator, asymptotic consistency

In this work, we present a nonparametric method for estimating the conditional density associated to the jump rate of a piecewise-deterministic Markov process. In our framework, the estimation needs only one observation of the process within a long time interval. Our method relies on a generalization of Aalen?s multiplicative intensity model. We prove the uniform consistency of our estimator, under some reasonable assumptions related to the primitive characteristics of the process. A simulation study illustrates the behavior of our estimator.

It has been accepted for publication in Scandinavian Journal of Statistics [17].

6.3. Finite Linear Programming Approximations of constrained discounted Markov decision processes

Participant: François Dufour.

Constrained Markov decision processes, linear programming approach to control problems, quantization, approximation of Markov decision processes

We consider a Markov decision process (MDP) with constraints under the total expected discounted cost optimality criterion. We are interested in proposing approximation methods of the optimal value of this constrained MDP. To this end, starting from the linear programming (LP) formulation of the constrained MDP (on an infinite-dimensional space of measures), we propose a finite state approximation of this LP problem. This is achieved by suitably approximating a probability measure underlying the random transitions of the dynamics of the system. Explicit convergence orders of the approximations of the optimal constrained cost are obtained. By exploiting convexity properties of the class of relaxed controls, we reduce the LP formulation of the constrained MDP to a finite-dimensional static optimization problem, that can be used to obtain explicit numerical approximations of the corresponding optimal constrained cost. A numerical application illustrates our theoretical results.

These results have been obtained in collaboration with Tomas Prieto-Rumeau, Department of Statistics and Operations Research, UNED, Madrid, Spain.

It has been published in SIAM Journal of Control and Optimization [25].

6.4. Stochastic Approximations of Constrained Discounted Markov Decision Processes

Participant: François Dufour.

Constrained Markov decision processes; Linear programming approach to control problems; Approximation of Markov decision processes

We consider a discrete-time constrained Markov decision process under the discounted cost optimality criterion. The state and action spaces are assumed to be Borel spaces, while the cost and constraint functions might be unbounded. We are interested in approximating numerically the optimal discounted constrained cost. To this end, we suppose that the transition kernel of the Markov decision process is absolutely continuous with respect to some probability measure μ. Then, by solving the linear programming formulation of a constrained control problem related to the empirical probability measure μ_n of μ, we obtain the corresponding approximation of the optimal constrained cost. We derive a concentration inequality which gives bounds on the probability that the estimation error is larger than some given constant. This bound is shown to decrease exponentially in n. Our theoretical results are illustrated with a numerical application based on a stochastic version of the Beverton-Holt population model.

These results have been obtained in collaboration with Tomas Prieto-Rumeau, Department of Statistics and Operations Research, UNED, Madrid, Spain.

It has been accepted for publication in Journal of Mathematical Analysis and Applications [26].

6.5. The expected total cost criterion for Markov decision processes under constraints

Participant: François Dufour.

Markov decision process, expected total cost criterion, constraints, linear programming, occupation measure

In this work, we study discrete-time Markov decision processes (MDPs) with constraints when all the objectives have the same form of expected total cost over the infinite time horizon. Our objective is to analyze this problem by using the linear programming approach. Under some technical hypotheses, it is shown that if there exists an optimal solution for the associated linear program then there exists a randomized stationary policy which is optimal for the MDP, and that the optimal value of the linear program coincides with the optimal value of the constrained control problem. A second important result states that the set of randomized stationary policies provides a sufficient set for solving this MDP. It is important to notice that, in contrast with the classical results of the literature, we do not assume the MDP to be transient or absorbing. More importantly, we do not impose the cost functions to be non-negative or to be bounded below. Several examples are presented to illustrate our results.

These results have been obtained in collaboration with Alexey Piunovskiy from Department. of Mathematical Sciences.

It has been published in Advances in Applied Probability [24].

6.6. Optimal stopping for piecewise-deterministic Markov processes and applications

Participants: Adrien Brandejsky, Benoîte de Saporta, François Dufour, Huilong Zhang.

We worked further on numerical methods for optimal stopping of PDMPs. On the one hand, we applied our numerical method to compute an optimal maintenance date to the test case of the heated hold-up tank. The system consists of a tank containing a fluid whose level is controlled by three components: two inlet pumps and one outlet valve. A thermal power source heats up the fluid. The failure rates of the components depends on the temperature, the position of the three components monitors the liquid level in the tank and the liquid level determines the temperature. Therefore, this system can be modeled by a hybrid process where the discrete (components) and continuous (level, temperature) parts interact in a closed loop. We model the system by a piecewise deterministic Markov process, propose and implement a numerical method to compute the optimal maintenance date to repair the components before the total failure of the system. This work is published in [30].

On the other hand, we investigated the optimal stopping problem under partial observations for PDMPs. We first obtain a recursive formulation of the optimal filter process and derive the dynamic programming equation of the partially observed optimal stopping problem. Then, we propose a numerical method, based on the quantization of the discrete-time filter process and the inter-jump times, to approximate the value function and to compute an ϵ-optimal stopping time. We prove the convergence of the algorithms and bound the rates of convergence. This work is published in [20].

6.7. Stochastic control for underwater optimal trajectories

Participants: Benoîte de Saporta, François Dufour, Huilong Zhang.

This work aims to compute optimal trajectories for underwater vehicles evolving in a given environment to accomplish some tasks. This is an optimal control problem. In real context, available inputs are not perfectly known. Hence a stochastic approach seems to be needed, coupled with the outputs of the tracking algorithms. Markov decision processes (MDPs) constitute a general family of controlled stochastic processes suitable for the modeling of sequential decision-making problems. The analysis of MDPs leads to mathematical and computational problems. The corresponding theory has reached a rather high degree of maturity, although the classical tools (such as value iteration, policy iteration, linear programming, and their various extensions) are generally hardly applicable in practice. Hence, solving MDPs numerically is an awkward and important problem. The method is applied to control a submarine which wants to well detect one or several targets and only has the information given by the tracking algorithms from the sonar observations [47].

6.8. Modeling of cell division data

Participants: Benoîte de Saporta, Anne Gégout-Petit.

This work is in collaboration with Laurence Marsalle (Univ. Lille 1).

A rigorous methodology is proposed to study cell division data consisting in several observed genealogical trees of possibly different shapes. The procedure takes into account missing observations, data from different trees, as well as the dependence structure within genealogical trees. Its main new feature is the joint use of all available information from several data sets instead of single data set estimation, to avoid the drawbacks of low accuracy for estimators or low power for tests on small single trees. The data is modeled by an asymmetric bifurcating autoregressive process and possibly missing observations are taken into account by modeling the genealogies with a two-type Galton-Watson process. Least-squares estimators of the unknown parameters of the processes are given and symmetry tests are derived. Results are applied on real data of Escherichia coli division and an empirical study of the convergence rates of the estimators and power of the tests is conducted on simulated data. This work is to appear in [29].

We have also presented a new model of asymmetric bifurcating autoregressive process with random coefficients. We couple this model with a Galton-Watson tree to take into account possibly missing observations. We propose least-squares estimators for the various parameters of the model and prove their consistency, with a convergence rate, and asymptotic normality. We use both the bifurcating Markov chain and martingale approaches and derive new results in both these frameworks. This work is to appear in [28].

6.9. Numerical method for the filtering of Markov jump linear systems

Participants: Benoîte de Saporta, Eduardo Costa.

We are interested in efficient pre-computations of the solutions of Markov switching Riccati equations. These equations are matrix-valued and naturally arise in control or filtering problems for Markov jump linear systems. It is crucial for applications to be able to compute the filter in real time, although the solutions to Riccati equations are slow to compute. Hence the need for pre-computations, taking into account the random possible changes of regimes. We propose a numerical method based on the discretization by quantization of the underlying Markov chain.

6.10. Optimization of the assembly line of the future European launcher

Participants: Benoîte de Saporta, François Dufour, Christophe Nivot.

In collaboration with Astrium space transportation, we have started working on the optimization of the assembly line of the future European launcher. We have started with a simplified model with five components to be assembled in workshops liable to breakdowns. We have modeled the problem using the Markov Decision Processes (MDP) framework and built a simulator of the process in order to run an optimization procedure

6.11. A variable clustering approach for the typology of units: a survey on farming and environment

Participants: Jérôme Saracco, Marie Chavent.

A survey on farming and environment dealing with the current transformations of the farmer job is considered. We propose to replace the usual data mining strategy which consists of applying Multiple Correspondence Analysis by a variable clustering approach. Clustering of variables aims at lumping together variables which are strongly related to each other and thus bring the same information. The ClustOfVar approach used in this paper provides at the same time groups of variables and their associated synthetic variables. In this algorithm, the homogeneity criterion of a cluster is defined by the squared Pearson correlation for the quantitative variables and by the correlation ratio for the qualitative variables. The step of variable clustering enables to get synthetic variables that can be read as a gradient. In our case study, values correspond to some relevant groupings of categories. This enables to interpret and name easily the synthetic variables. Trends in the opinion of farmers are thus highlighted with the variable clustering approach. Then we clarify these first results by applying a clustering method on the scores of the individuals measured by the synthetic variables. At the sociological level, the supply provided by the synthetic variables to interpret the clusters of farmers is obvious.

These results have been obtained in collaboration with Vanessa Kuentz from Irstea, UR ADBX.

They have been published in Journal de la Société Française de Statistique [31].

6.12. Multiple Facctorial Analysis for mixed data type

Participants: Jérôme Saracco, Marie Chavent, Amaury Labenne.

Multiple Factor Analysis (MFA) originally proposed by Escofier and Pages in 1982 is a method dedicated to the study of a set of n individuals described by groups of quantitative variables. Later, this method was extended to take into account groups of qualitative variables (Pages, 1983) then simultaneously quantitative groups and qualitative groups (Pages, 2002). However, this method does not currently take into account mixed groups, that is to say containing both quantitative and qualitative variables. The aim of our study is to propose sustainable development indicators by integrating the aspect of quality of life. For that, we are confronted with the analysis of groups of variables with quantitative and qualitative variables. In this work, we propose an extension of the MFA method, called MFAMIX, for the multiple factor analysis of mixed groups of variables. This approach relies on a combination of AFM and PCAMIX method that allows the analysis of mixed data. MFAMIX method is presented using a singular value decomposition and illustrated on socio-economic data about the quality of life.

These results have been obtained in collaboration with Vanessa Kuentz from Irstea, UR ADBX.

They have been have been presented in two national conferences [43], [41].

6.13. Detecting mental states of alertness with genetic algorithm variable selection

Participants: Marie Chavent, Laurent Vézard.

The objective of the present work is to develop a method able to automatically determine mental states of vigilance; i.e., a person's state of alertness. Such a task is relevant to diverse domains, where a person is expected or required to be in a particular state. For instance, pilots or medical staffs are expected to be in a highly alert state, and this method could help to detect possible problems. In this paper, an approach is developed to predict the state of alertness ("normal" or "relaxed") from the study of electroencephalographic signals (EEG) collected with a limited number of electrodes. The EEG of 58 participants in the two alertness states (116 records) were collected via a cap with 58 electrodes. After a data validation step, 19 subjects were retained for further analysis. A genetic algorithm was used to select an optimal subset of electrodes. Common spatial pattern (CSP) coupled to linear discriminant analysis (LDA) was used to build a decision rule and thus predict the alertness of the participants. Different subset sizes were investigated and the best result was obtained by considering 9 electrodes (correct classification rate of 73.68

These results have been obtained in collaboration with Pierrick Legrand from Alea Inria team and Leonardo Trujillo from Instituto Tecnologico de Tijuana.

This work has been presented in a international IEEEl conference [38].

6.14. ClustOfVar : an R package for dimension reduction via clustering of variables. Application in supervised classification and variable selection in gene expressions data

Participants: Marie Chavent, Jérôme Saracco.

The main goal of this work is to tackle the problem of dimension reduction for high-dimensional supervised classication. The motivation is to handle gene expression data. The proposed method works in 2 steps. First, one eliminates redundancy using clustering of variables, based on the R-package ClustOfVar. This first step is only based on the exploratory variables (genes). Second, the synthetic variables (summarizing the clusters obtained at the first step) are used to construct a classifier (e.g. logistic regression, LDA, random forests). We stress that the first step reduces the dimension and gives linear combinations of original variables (synthetic variables). This step can be considered as an alternative to PCA. A selection of predictors (synthetic variables) in the second step gives a set of relevant original variables (genes). Numerical performances of the proposed procedure are evaluated on gene expression datasets. We compare our methodology with LASSO and sparse PLS discriminant analysis on these datasets.

This work is a collaboration with Robin Genuer from SISTM Inria team and Benoit Liquet from University of Queensland.

This work has been presented in a international workshop on Statistical Methods for (post)-Genomics Data (SMPGD 2013) [42].

6.15. A sliced inverse regression approach for data stream

Participants: Jérôme Saracco, Marie Chavent.

This work is in collaboration with Stéphane Girard (Inria Grenoble Alpes), Benoît Liquet (MRC, Cambridge University), Vanessa Kuentz (Irstea) and Thi Mong Gnoc Nguyen (Univ. de Strasbourg).

In this work, we focus on data arriving sequentially by blocks in a stream. A semiparametric regression model involving a common EDR (Effective Dimension Reduction) direction is assumed in each block. Our goal is to estimate this direction at each arrival of a new block. A simple direct approach consists of pooling all the observed blocks and estimating the EDR direction by the SIR (Sliced Inverse Regression) method. But in practice, some disadvantages appear such as the storage of the blocks and the running time for large sample sizes. To overcome these drawbacks, we propose an adaptive SIR estimator of based on the optimization of a quality measure. The corresponding approach is faster both in terms of computational complexity and running time, and provides data storage benefits. The consistency of our estimator is established and its asymptotic distribution is given. An extension to multiple indices model is proposed. A graphical tool is also provided in order to detect changes in the underlying model, i.e., drift in the EDR direction or aberrant blocks in the data stream. A simulation study illustrates the numerical behavior of our estimator. Finally, an application to real data concerning the estimation of physical properties of the Mars surface is presented.

This work is to appear in [21].

6.16. Comparison of Kernel Density Estimators with Assumption on Number of Modes

Participant: Jérôme Saracco.

This work is in collaboration with Bernard Bercu (Univ. Bretagne Sud) and Thi Mong Gnoc Nguyen (Univ. de Strasbourg).

In this work, we investigate the asymptotic behavior of the Nadaraya-Watson estimator for the estimation of the regression function in a semiparametric regression model. On the one hand, we make use of the recursive version of the sliced inverse regression method for the estimation of the unknown parameter of the model. On the other hand, we implement a recursive Nadaraya-Watson procedure for the estimation of the regression function which takes into account the previous estimation of the parameter of the semiparametric regression model. We establish the almost sure convergence as well as the asymptotic normality for our Nadaraya-Watson estimator. We also illustrate our semiparametric estimation procedure on simulated data.

This work is to appear in [19].

6.17. Comparison of Kernel Density Estimators with Assumption on Number of Modes

Participants: Jérôme Saracco, Raphaël Coudret.

This work is in collaboration with Gilles Durrieu (Univ. Bretagne Sud).

A data-driven bandwidth choice for a kernel density estimator called critical bandwidth is investigated. This procedure allows the estimation to have as many modes as assumed for the density to estimate. Both Gaussian and uniform kernels are considered. For the Gaussian kernel, asymptotic results are given. For the uniform kernel, an argument against these properties is mentioned. These theoretical results are illustrated with a simulation study which compare the kernel estimators that rely on critical bandwidth with another one which uses a plug-in method to select its bandwidth. An estimator that consists in estimates of density contour clusters and takes assumptions on number of modes into account is also considered. Finally, the methodology is illustrated using environment monitoring data.

This work is to appear in [22].

6.18. Comparison of sliced inverse regression approaches for underdetermined cases

Participants: Jérôme Saracco, Raphaël Coudret.

This work is in collaboration with Benoît Liquet (MRC, Cambridge University).

Among methods to analyze high-dimensional data, the sliced inverse regression (SIR) is of particular interest for non-linear relations between the dependent variable and some indices of the covariate. When the dimension of the covariate is greater than the number of observations, classical versions of SIR cannot be applied. Various upgrades were then proposed to tackle this issue such as regularized SIR (RSIR) and sparse ridge SIR (SR-SIR), to estimate the parameters of the underlying model and to select variables of interest. In this paper, we introduce two new estimation methods respectively based on the QZ algorithm and on the Moore-Penrose pseudo-inverse. We also describe a new selection procedure of the most relevant components of the covariate that relies on a proximity criterion between submodels and the initial one. These approaches are compared with RSIR and SR-SIR in a simulation study. Finally we applied SIR-QZ and the associated selection procedure to a genetic dataset in order to find markers that are linked to the expression of a gene. These markers are called expression quantitative trait loci (eQTL).

This work was presented in a national conference [23] and is to appear in [37].

6.19. Conditional Quantile Estimationthrough Optimal Quantization

Participants: Jérôme Saracco, Isabelle Charlier.

This work is in collaboration with Davy Paindaveine (Univ. Libre de Bruxelles).

In this work, we construct a nonparametric estimator of conditional quantiles of Y given X via optimal quantization. In a first step, we propose to approximate conditional quantiles thanks to optimal quantization in L^p-norm, consisting in discretizing X and Y thanks to some optimal grids of size N. We state a result of convergence of this approximation toward the true conditional quantile. The estimator was implemented in **R** in order to evaluate its numerical behavior and to compare it with existing estimators. A simulation study illustrates the good behavior of our estimator. The practical choice of N is discussed. We apply our approach to a real data set.

This work was presented in a national conference [35].

6.20. Estimation of water consumption based on survey techniques using an automatic meter reading sample

Participant: Jérôme Saracco.

This work is in collaboration with Karim Claudio (LyRE), Vincent Couallier (Univ. de Bordeaux) and Yves Le Gat (Irstea).

Automatic water meters reading are, nowadays, the best technology for real time knowledge of water consumption. At an hydraulic sector scale, a complete equipment permits to know the total consumption of a finite size population, for a time scale as small as the hour. However its cost for generalization is sometimes unbearable for the collectivity, for whom sampling techniques have to be set up. In a objective of a total consumption estimation, this article describes and compares standard methods of survey techniques and propose to retain a methodology for implementation of an operational sample and to calibrate the corresponding total estimator.

This work was presented in a national conference [36] and an associated paper is currently in revision.

6.21. Hidden Markov Model for the detection of a degraded operating mode of optronic equipment

Participants: Camille Baysse, Anne Gégout-Petit, Jérôme Saracco.

This work is in collaboration with Didier Bihannic (Thales Optronics) and Michel Prenat (Thales Optronics).

As part of optimizing the reliability, Thales Optronics now includes systems that examine the state of its equipment. The aim of this work is to use hidden Markov Model to detect as soon as possible a change of state of optronic equipment in order to propose maintenance before failure. For this, we carefully observe the dynamic of a variable called "cool down time" and noted Tmf, which reflects the state of the cooling system. Indeed, the Tmf is an observation of the hidden state of the system. This one is modeled by a Markov chain and the Tmf is a noisy function of it. Thanks to filtering equations, we obtain results on the probability that an appliance is in degraded state at time t, knowing the history of the Tmf until this moment. We have evaluated the numerical behavior of our approach on simulated data. Then we have applied this methodology on our real data and we have checked that the results are consistent with the reality. This method can be implemented in a HUMS (Health and Usage Monitoring System). This simple example of HUMS would allow the Thales Optronics Company to improve its maintenance system. This company will be able to recall appliances which are estimated to be in degraded state and do not control too early those estimated in stable state.

This work is to appear in [18].

6.22. A new sliced inverse regression method for multivariate response

Participants: Jérôme Saracco, Raphaël Coudret.

This work is in collaboration with Stéphane Girard (Inria Grenoble Alpes).

We consider a semiparametric regression model of a q-dimensional multivariate response y on a p-dimensional covariate x. In this paper, a new approach is proposed based on sliced inverse regression for estimating the effective dimension reduction (EDR) space without requiring a prespecified parametric model. The convergence at rate $\sqrt{n}$ of the estimated EDR space is shown. We discuss the choice of the dimension of the EDR space. The numerical performance of the proposed multivariate SIR method is illustrated on a simulation study. Moreover, we provide a way to cluster components of y related to the same EDR space. One can thus apply properly multivariate SIR on each cluster instead of blindly applying multivariate SIR on all components of y. An application to hyperspectral data is provided.

This work is currently under revision, see [48].

6.23. An introduction to dimension reduction in nonparametric kernel regression

Participant: Jérôme Saracco.

This work is in collaboration with Stéphane Girard (Inria Grenoble Alpes).

Nonparametric regression is a powerful tool to estimate nonlinear relations between some predictors and a response variable. However, when the number of predictors is high, nonparametric estimators may suffer from the curse of dimensionality. In this chapter, we show how a dimension reduction method (namely Sliced Inverse Regression) can be combined with nonparametric kernel regression to overcome this drawback. The methods are illustrated both on simulated datasets as well as on an astronomy dataset using the **R** software.

This work was presented in "School in Astrostatistics" (Annecy, October, 21-25, 2013) and is to appear as a chapter in book intilted *Methods and Applications of Regression in Astrophysics* in 2014.

MATHRISK Project-Team

6. New Results

6.1. Credit risk

Participants: Aurélien Alfonsi, Céline Labart, Jérôme Lelong.

We have ended our study on stochastic local intensity model. We have shown by the mean of a particles system that this model is well defined and have obtained an efficient way to perform Monte-Carlo algorithms for this model.

6.2. Liquidity risk

Participants: Aurélien Alfonsi, A. Schied.

A. Alfonsi and A. Schied (Mannheim University) are working on price impact models that describe how the price is modified by large trades. The paper together with J. Acevedo on a time-dependent price impact is now accepted for publication. With A. Schied and F. Klöck [45], we have studied the cross price impact between different assets and identified conditions on the resilience of this impact that avoid manipulations strategies. With P. Blanc, we are working on the optimal execution problem when there are many large traders that modify the price.

6.3. Systemic Risk

Participants: Andreea Minca, Agnès Sulem.

We are working on the theory of the stochastic control of financial networks.

In two related articles, we find the optimal strategy of a government who seeks to make equity infusions in a banking system prone to insolvency and to bank runs. The first article combines stochastic control and the random graph representation of the financial system developed in Andreea's thesis. The second article combines the network representation of a financial system and the solvency-based mechanism of contagion with another potent source of distress, which is funding illiquidity [31] and [60].

6.4. Estimation of the parameters of a Wishart process

Participants: Aurélien Alfonsi, Ahmed Kebaier, Clément Rey.

This research has started this year together with the thesis of Clément Rey. We are studying the Maximum Likelihood Estimator for the Wishart processes and in particular its convergence in the ergodic and the non ergodic case.

6.5. An Affine term structure model for interest rates that involve Wishart diffusions

Participants: Aurélien Alfonsi, E. Palidda.

Affine term structure models (Dai and Singleton, Duffie, ...) consider vector affine diffusions. Here, we would like to extend this model by including some Wishart dynamics, and to get a model that could better fit the market. We also develop some numerical pricing methods for this model to make its implementation possible.

6.6. Applications of optimal transport

Participants: Aurélien Alfonsi, Benjamin Jourdain, Arturo Kohatsu-Higa.

A. Alfonsi and B. Jourdain study the Wasserstein distance between two probability measures in dimension n sharing the same copula C. The image of the probability measure dC by the vectors of pseudo-inverses of marginal distributions is a natural generalization of the coupling known to be optimal in dimension $n = 1$. In dimension $n > 1$, it turns out that for cost functions equal to the p-th power of the L^q norm, this coupling is optimal only when $p = q$ i.e. when the cost function may be decomposed as the sum of coordinate-wise costs.

As another application of optimal transport, they are working with A. Kohatsu-Higa on the uniform in time estimation of the Wasserstein distance between the time-marginals of an elliptic diffusion and its Euler scheme. To generalize in higher dimension the result that they obtained previously in dimension one using the optimality of the explicit inverse transform, they compute the derivative of the Wasserstein distance with respect to the time variable thanks to the theory developped by Ambrosio Gigli and Savare. The abstract properties of the optimal coupling between the time marginals then enable them to estimate this time derivative.

6.7. Capital distribution and portfolio performance in the mean-field Atlas model

Participants: Benjamin Jourdain, J. Reygner.

B. Jourdain and J. Reygner study a mean-field version of rank-based models of equity markets, introduced by Fernholz in the framework of stochastic portfolio theory. They first obtain an asymptotic description of the market when the number of companies grows to infinity. They then discuss the long-term capital distribution in this asymptotic model, as well as the performance of simple portfolio rules. In particular, they highlight the influence of the volatility structure of the model on the growth rates of portfolios.

6.8. Public Private Partnerships

Participants: Gilles Edouard Espinosa, Caroline Hillairet, Benjamin Jourdain, Monique Pontier.

With Gilles Edouard Espinosa, Caroline Hillairet and Monique Pontier, Benjamin Jourdain is interested in the problem of outsourcing the debt for a big investment, according two situations: either the firm outsources both the investment (and the associated debt) and the exploitation to a private consortium, or the firm supports the debt and the investment but outsources the exploitation. They prove the existence of Stackelberg and Nash equilibria between the firm and the private consortium, in both situations. They compare the benefits of these contracts.They conclude with a study of what happens in case of incomplete information, in the sense that the risk aversion coefficient of each partner may be unknown by the other partner [51].

6.9. Backward Stochastic (Partial) Differential equations with jumps and stochastic control

Participants: Roxana-Larisa Dumitrescu, Marie-Claire Quenez, Agnès Sulem.

We have studied optimization problems for BSDEs with jumps, optimal stopping for dynamic risk measures induced by BSDEs with jumps and associated reflected BSDEs, and generalized Dynkin games associated to double barriers reflected BSDEs with jumps [32], [38], [42]. A. Sulem, with B. Øksendal and T. Zhang has also studied optimal stopping for Stochastic Partial Differential equations and associated reflected SPDEs [34], and optimal control of Forward-Backward SDEs [54].

6.10. Utility maximization and Arbitrage Theory

Participants: Claudio Fontana, Bernt Øksendal, Agnès Sulem.

B. Øksendal and A. Sulem have contributed to the issue of robust utility maximization in jump diffusion markets via a stochastic maximum approach and the links with robust duality [53].

In the period January - October 2013, the main subject of investigation of C. Fontana has been arbitrage theory, with a special emphasis on no-arbitrage conditions weaker than the classical notion of No Free Lunch with Vanishing Risk (NFLVR). In particular, in the context of financial market models based on diffusion processes (see [35]), we have provided a characterization of several no-arbitrage conditions as well as a generalization of the second fundamental theorem of asset pricing. In the context of jump-diffusion models under partial information (see [25]), we have studied the relation between market viability (in the sense of solvability of portfolio optimization problems) and the existence of a martingale measure given by the marginal utility of terminal wealth, without a-priori assuming no-arbitrage restrictions on the model. Finally, in the paper [41], we have provided a critical analysis of the paper Arbitrage, Approximate Arbitrage and the Fundamental Theorem of Asset Pricing (Wong & Heyde, 2010), where the authors aim at proposing an original and simple proof of the fundamental theorem of asset pricing in the context of incomplete diffusion-based models. We have shown that the method of Wong & Heyde (2010) can only work in the well-known case of complete markets, exhibiting an explicit counterexample.

6.11. Regularity of probability laws using an interpolation method

Participant: Vlad Bally.

This work was motivated by previous papers of Nicolas Fournier, J. Printemps, E. Clément, A. Debusche and of myself, concerning the regularity of the law of the solutions of some equations with coefficients with little regularity - for example diffusion processes with Hölder coefficients (but also many other examples including jump type equations, Bolzmann equation or Stochastic PDE's). Since we do not have sufficient regularity the usual approach by Malliavin calculus fails in this framework. Then one may use an alternative idea which roughly speaking is the following: We approximate the law of the random variable X (the solution of the equation at hand) by a sequence $X(n)$ of random variables which are smooth and consequently we are able to establish integration by parts formulas for $X(n)$ and we are able to obtain the absolutely continuity of the law of $X(n)$ and to establish estimates for the density of the law of $X(n)$ and for its derivatives. Notice that the derivatives of the densities of $X(n)$ generally blow up - so we can not derive directly results concerning the density of the law of X. But, if the speed of convergence of $X(n)$ to X is stronger than the blow up, then we may obtain results concerning the density of the law of X. It turns out that this approach fits in the framework of interpolation spaces and that the criterion of regularity for the law of X amounts to the characterization of an interpolation space between a space of distributions and a space of smooth functions. Although the theory of interpolation spaces is very well developed and one already know to characterize the interpolation spaces for Sobolev spaces of positive and negative indices, we have not found in the (huge) literature a result which covers the problem we are concerned with. So, although our result may be viewed as an interpolation result, it is a new one. The above work is treated in the paper [62] (in collaboration with Lucia Caramellino). As an application we discussed in [48] the regularity of the law of a Wiener functional under a Hörmander type non degeneracy condition.

6.12. A stochastic parametric representation for the density of a Markov process

Participant: Vlad Bally.

Classical results in the PDE theory (due to A. Friedmann) assert that, under uniform ellipticity conditions, the law of a diffusion process has a continuous density (the approach of A. Friedmann is analytical and concerns PDE's instead of the corresponding diffusion process). The method developed by A. Friedmann becomes well known as the "parametric method". In collaboration with A. Kohatzu Higa [49] we gave a probabilistic approach which represents the probabilistic counterpart of the parametric method. We obtained a probabilistic representation for the density of the law of the solution of a SDE and more generaly, for a class of Markov processes including solutions of jump type SDE's. This representation may be considered as a perfect simulation scheme and so represents a starting point for Monte Carlo simulation. However the random variable which appears in the stochastic representation has infinite variance, so direct simulation gives unstable results (as some preliminary tests have proved). In order to obtain an efficient simulation scheme some more work on the reduction of variance has to be done.

6.13. Regularity of probability laws using an interpolation method

Participant: Vlad Bally.

The distance between two density functions and convergence in total variation. In collaboration with Lucia Caramellino we obtained estimates of the distance between the densities of the law of two random variables using an abstract variant of Malliavin calculus. We used these estimates in order to study the convergence in total variation of a sequence of random variables. This has been done in [47]. We are now working on more specific examples concerning the Central Limit Theorem. In the last years the convergence in entropy distance and in total variation distance for several variants of the CLT has been considered in papers of S. Bobkov, F. Gotze, G. Peccati, Y. Nourdin, D. Nualart and G. Polly. So this seems to be a very active research area. Moreover, in an working paper in collaboration with my Phd student R. Clement, we use the same methods in order to study the total variation distance between two Markov semigroups and in particular for approximation schemes. A special interest is devoted to higher order schemes - as for example the Victoire Nyomia scheme.

REGULARITY Project-Team

6. New Results

6.1. Stochastic integration with respect to the Rosenblatt process.

Participant: Benjamin Arras.

From a theoretical perspective to more concrete applications, fractional Brownian motion (fbm) is a fruitful and rich mathematical object. From its stochastic analysis, initiated during the nineties, several theories of stochastic integration have emerged so far. Indeed, fbm is, in general, not a semimartingale neither a Markov process. These theories rely on different properties of the stochastic integrator process and are then of different natures. Despite the quite large number of these strategies, we can group them into two fundamentally distinct categories: the pathwise and the probabilistic approaches. The probabilistic one requires highly evolved stochastic analysis tools. Indeed, the Malliavin calculus as well as Hida's distribution theory have been used in order to define stochastic integration with respect to fractional Brownian motion ([56], [52]) and more general Gaussian processes ([47]). Moreover, fbm belongs to an important class of stochastic processes, namely, the Hermite processes. This class appears in non-central limit theorems for processes defined as integrals or partial sums of non-linear functionals of stationary Gaussian sequences with long-range dependence (see [57]). They admit the following representation for all $d \geq 1$:

$$\forall t > 0 \quad Y_t^{H,d} = c(H_0) \int_{\mathbb{R}} ... \int_{\mathbb{R}} \left(\int_0^t \prod_{j=1}^{d} (s - x_j)_+^{H_0 - 1} ds \right) dB_{x_1} ... dB_{x_d}$$

where $c(H_0)$ is a normalizing constant such that $\mathbb{E}[|Y_1^{H,d}|^2] = 1$ and $H_0 = \frac{1}{2} + \frac{H-1}{d}$ with $H \in (\frac{1}{2}, 1)$. For $d = 1$, one recovers fractional Brownian motion. These processes share many properties with fbm. Namely, they are H-self-similar processes with stationary increments. They possess the same covariance structure, exhibit long range-dependence and their sample paths are almost-surely δ-Hölder continuous, for every $\delta < H$. For $d = 2$, the process is called the Rosenblatt process. This process has received lots of interest in the past and more recent years. Stochastic calculus with respect to the Rosenblatt process has been developped in [73] from both, the pathwise type calculus and Malliavin calculus points of view. Even if these two approaches are successful in order to define a stochastic integral with respect to the Rosenblatt process, the Malliavin calculus one fails to give an Itô's formula for the Rosenblatt process in the divergence sense. In [42], by means of white noise distribution theory, we obtain the following result:

Theorem: Let $(a, b) \in \mathbb{R}_+^*$ such that $a \leq b < \infty$. Let F be an entire analytic function of the complex variable verifying:

$$\exists N \in \mathbb{N}, \exists C > 0, \forall z \in \mathbb{C} \quad |F(z)| \leq C(1 + |z|)^N \exp(\frac{1}{\sqrt{2} b^H} |\Im(z)|)$$

Then, we have in $(S)^*$:

$$F(X_b^H) - F(X_a^H) = \int_a^b F^{(1)}(X_t^H) \diamond \dot{X}_t^H dt + \sum_{k=2}^{\infty} \left(H \kappa_k(X_1^H) \int_a^b \frac{t^{Hk-1}}{(k-1)!} F^{(k)}(X_t^H) dt + 2^k \int_a^b F^{(k)}(X_t^H) \diamond \dot{X}_t^{H,k} dt \right),$$

where $\{X_t^H\} = \{Y_t^{H,2}\}$, $\{\dot{X}_t^H\}$ is the Rosenblatt noise, $\{\kappa_k(X_1^H); k \geq 2\}$ the non-zero cumulants of the Rosenblatt distribution, $\diamond$ the Wick product and $\{\{X_t^{H,k}\} : k \geq 2\}$ a sequence of processes defined by:

$$\forall t \geq 0 \quad X_t^{H,k} = \int_{\mathbb{R}} \int_{\mathbb{R}} \underbrace{(...((f_t^H \otimes_1 f_t^H) \otimes_1 f_t^H)... \otimes_1 f_t^H)}_{k-1 \times \otimes_1}(x_1, x_2) dB_{x_1} dB_{x_2}$$

with $f_t^H(x_1, x_2) = c(H) \int_0^t \prod_{j=1}^2 (s - x_j)_+^{\frac{H}{2}-1} ds$ and $\otimes_1$ is the contraction of order 1.
Moreover, in the same setting, we obtain the following "isometry" result for the Rosenblatt noise integral of sufficiently "good" integrand processes:
Theorem: Let $\{\phi_t; t \in I\}$ be a stochastic process such that for all $t \in I$ (I an interval), $\phi_t \in (L^2)$ and such that the Rosenblatt noise integral of $\{\phi_t\}$ exists in $(S)^*$. Moreover, let us assume that:

$$\sum_{m=0}^{+\infty} (m+2)! \int_I \int_I |t-s|^{2(H-1)} < f_m(.,t); f_m(.,s) >_{L^2(\mathbb{R}^m)} dtds < +\infty,$$

where $\phi_t = \sum_{m=0}^{+\infty} I_m(f_m(.,t))$. Thus, we have:

$$\mathbb{E}[(\int_I \phi_t \diamond \dot{X}_t^H dt)^2] = H(2H-1) \int_I \int_I |t-s|^{2(H-1)} \mathbb{E}[\phi_t \phi_s] dsdt$$
$$+4\sqrt{\frac{H(2H-1)}{2}} \int_I \int_I |t-s|^{H-1} \mathbb{E}[D_{\sqrt{d(H)}\delta_s \circ I_+^{\frac{H}{2}}}(\phi_t) D_{\sqrt{d(H)}\delta_t \circ I_+^{\frac{H}{2}}}(\phi_s)] dsdt$$
$$+ \int_I \int_I \mathbb{E}[(D_{\sqrt{d(H)}\delta_s \circ I_+^{\frac{H}{2}}})^2(\phi_t)(D_{\sqrt{d(H)}\delta_t \circ I_+^{\frac{H}{2}}})^2(\phi_s)] dsdt,$$

where $D_{\sqrt{d(H)}\delta_s \circ I_+^{\frac{H}{2}}}$ is the derivative operator in the direction $\sqrt{d(H)}\delta_s \circ I_+^{\frac{H}{2}}$.
Finally, in the last section of [42], we compare our approach to the one of [73]. More specifically, we prove that the stochastic integral with respect to the Rosenblatt process built using Malliavin calculus corresponds with the Rosenblatt noise integral when both of them exist.
Proposition: Let $\{\phi_t; t \in [0;T]\}$ be a stochastic process such that $\phi \in L^2(\Omega; \mathcal{H}) \cap L^2([0,T]; \mathbb{D}^{2,2})$ and $\mathbb{E}[\int_0^T \int_0^T ||D_{s_1,s_2}\phi||_{\mathcal{H}}^2] ds_1 ds_2 < \infty$ where

$$\mathcal{H} = \{f : [0;T] \to \mathbb{R}; \int_0^T \int_0^T f(s)f(t)|t-s|^{2H-2} dsdt < \infty\}.$$

Then, $\{\phi_t\}$ is Skorohod integrable and $(S)^*$-integrable with respect to the Rosenblatt process, $\{Z_t^H\}_{t\in[0;T]}$, and we have:

$$\int_0^T \phi_t \delta Z_t^H = \int_0^T \phi_t \diamond \dot{Z}_t^H dt$$

6.2. Sample path properties of multifractional Brownian motion

Participants: Paul Balança, Erick Herbin [supervision].

In [50], we have investigated the geometry of the sample paths of multifractional Brownian motion. Several representations of mBm exist, including the classic integral form:

$$\forall t \in \mathbf{R}; \quad X_t = \frac{1}{\Gamma\left(H(t) + \frac{1}{2}\right)} \int_{\mathbf{R}} \left[(t-u)_+^{H(t)-1/2} - (-u)_+^{H(t)-1/2}\right] \mathrm{d}W_u,$$

where $H : \mathbf{R} \mapsto (0,1)$ is a continuous function. Interestingly, we observe that geometric properties obtained in the probabilistic literature usually rely on a key assumption on the behaviour of the Hurst function:

$$H \text{ is a } \beta\text{-Hölder continuous function such that } \forall t \in \mathbf{R},\ H(t) < \beta. \qquad (\mathcal{H}_0) \tag{25}$$

Under the previous hypothesis, the local regularity of the mBm at t corresponds to the geometry of a fractional Brownian motion of parameter $H(t)$. Nevertheless, it has been shown in [15] that when this assumption does not hold, the sample path properties are not as simple and straightforward. More precisely, the latter has proved that the Hölder exponents satisfy at every $t \in \mathbf{R}$:

$$\alpha_{X,t} = H(t) \wedge \alpha_{H,t} \quad \text{and} \quad \widetilde{\alpha}_{X,t} = H(t) \wedge \widetilde{\alpha}_{H,t} \quad \text{a.s.} \tag{26}$$

This result has been recently improved in [48], observing that the pointwise exponent can even be random under some assumptions on H.

Therefore, the main goal of this work was to obtain a more complete characterization of the geometry of the general mBm. We have first focused on the Hölder regularity of the sample paths, using for this purpose a deterministic representation of the fractional Brownian field:

$$B^{\pm}(t,H) = \frac{\pm 1}{\Gamma\left(H-\frac{1}{2}\right)} \int_{\mathbf{R}} B_u \left[(t-u)_{\pm}^{H-3/2} - (-u)_{\pm}^{H-3/2} \right] \mathrm{d}u, \tag{27}$$

where $H \geq 1/2$ and B is a continuous Brownian motion. Hence, observing that the mBm almost surely corresponds to the fractional integration of a Brownian motion, we have been able to use the 2-microlocal formalism and its interesting connections with fractional operators. As a consequence, we have proved that the pointwise exponent of the mBm almost surely satisfies:

$$\forall t \in \mathbf{R}; \quad \alpha_{X,t} = H(t) \wedge m_{t,H(t)} \alpha_{H,t}, \tag{28}$$

where $m_{t,H(t)}$ is defined as the multiplicity of the fractional Brownian field at (t,H), i.e.

$$m_{t,H} = \inf \left\{ k \in \mathbf{N} \setminus \{0\} : \partial_H^k B(t,H) \neq 0 \right\}.$$

We have also been able to obtain some uniform lower bounds on the 2-microlocal frontier, which are optimal under some mild assumptions on the Hurst function.

The second direction of our study has concerned the fractal dimension of the graph of the mBm. Interestingly, and on the contrary to fBm, we have to distinguish the Box and Hausdorff dimensions in our result. The first happens to be the easiest one to study and is closely related to the geometry of H itself. Therefore, with probability one,

$$\forall t \in \mathbf{R} \setminus \{0\}; \quad \dim_{\mathrm{B},t} \mathrm{Gr}(X) = (2 - H(t)) \vee \dim_{\mathrm{B},t} \mathrm{Gr}(H), \tag{29}$$

where $\dim_{\mathrm{B},t}$ denotes the localized Box dimension at t.

To study the Hausdorff dimension the graph, we need a slightly different approach which makes use of parabolic Hausdorff dimension. We first define for all $t \in \mathbf{R}$ a *parabolic metric* ϱ_H on $\mathbf{R}^2$, with $H > 0$: $\varrho_H((u,x);(v,y)) := \max\left(|u-v|^H, |x-y|\right)$. For any set $A \subset \mathbf{R}^2$, we denote by $\dim_{\mathcal{H}}(A;\varrho_H)$ the *parabolic Hausdorff dimension* of A. It is defined similarly to the classic Hausdorff dimension using covering balls relatively to the metric ϱ_H, i.e. it corresponds to the infimum of $s \geq 0$ for which

$$\liminf_{\delta \to 0} \left\{ \sum_{i=0}^{\infty} \operatorname{diam}(O_i;\varrho_H)^s : (O_i)_{i\in N} \text{ is a } \delta\text{-cover of } A \right\} < \infty$$

Studying the local Hausdorff dimension of the graph of the mBm, we have proved that with probability one

$$\forall t \in \mathbf{R} \setminus \{0\}; \quad \dim_{\mathrm{H},t} \operatorname{Gr}(X) = 1 + H(t)\left(\dim_{\mathrm{H},t}\left(\operatorname{Gr}(H);\varrho_{H(t)}\right) - 1\right). \tag{30}$$

Even though this result might seem counter-intuitive, it can be checked that it induced the classic equality $\dim_{\mathrm{H},t} \operatorname{Gr}(X) = 2 - H(t)$ when the mBm satisfies the assumption $\mathcal{H}_0$. Interestingly, we observe that a similar expression has also emerged recently in the study [70] of the Hausdorff dimension of a fractional Brownian motion with variable drift. Finally, we also note this result can also been extended to images of fractal sets by the multifractional Brownian motion.

6.3. Large Deviations Inequalities

Participant: Xiequan Fan.

Let $(\xi_i)_{i=1,\ldots,n}$ be a sequence of independent and centered random variables satisfying Bernstein's condition, for a constant $\varepsilon > 0$,

$$|\mathbb{E}\xi_i^k| \leq \frac{1}{2}k!\varepsilon^{k-2}\mathbb{E}\xi_i^2, \quad \text{for all } k \geq 2 \text{ and all } i = 1,\ldots,n. \tag{31}$$

Denote by

$$S_n = \sum_{i=1}^{n} \xi_i \quad \text{and} \quad \sigma^2 = \sum_{i=1}^{n} \mathbb{E}\xi_i^2. \tag{32}$$

The well-known Bernstein inequality (1946) states that, for all $x > 0$,

$$\mathbb{P}(S_n > x\sigma) \leq \inf_{\lambda \geq 0} \mathbb{E}e^{\lambda(S_n - x\sigma)}. \tag{33}$$

In the i.i.d. case, Cramér (1938) has established a large deviation expansion under the condition $\mathbb{E}e^{|\xi_1|} < \infty$. For all $0 \leq x = o(\sqrt{n})$, one has

$$\frac{\mathbb{P}(S_n > x\sigma)}{1 - \Phi(x)} = e^{\frac{x^3}{\sqrt{n}}\lambda\left(\frac{x}{\sqrt{n}}\right)}\left[1 + O\left(\frac{1+x}{\sqrt{n}}\right)\right], \quad n \to \infty, \tag{34}$$

where $\lambda(\cdot) = c_1 + c_2\frac{x}{\sqrt{n}} + \ldots$ is the Cramér series and the values $c_1, c_2, \ldots$ depend on the distribution of ξ_1.

Bahadur-Rao (1960) proved the following sharp large deviations similar to (15). Assume Cramér's condition. Then, for given $y > 0$, there is a constant c_y depending on the distribution of ξ_1 and y such that

$$\mathbb{P}\left(\frac{S_n}{n} > y\right) = \frac{\inf_{\lambda \geq 0}\mathbb{E}e^{\lambda(S_n - yn)}}{\sigma_y t_y \sqrt{2\pi n}}\left[1 + O\left(\frac{c_y}{n}\right)\right], \quad n \to \infty, \tag{35}$$

where t_y, σ_y and c_y depend on the distribution of ξ_1 and y.

We present an improvement on Bernstein's inequality. In particular, we establish a sharp large deviation expansion similar to the classical results of Cramér and Bahadur-Rao. The following theorem is our main result.

Theorem 0.1 Assume Bernstein's condition. Then, for all $0 \le x < \frac{1}{12}\frac{\sigma}{\varepsilon}$,

$$\mathbb{P}(S_n > x\sigma) = \inf_{\lambda \ge 0} \mathbb{E} e^{\lambda(S_n - x\sigma)} F\left(x, \frac{\varepsilon}{\sigma}\right), \tag{36}$$

where $\sqrt{2\pi}M(x)$ is the Mills ratio, the function

$$F\left(x, \frac{\varepsilon}{\sigma}\right) = M(x) + 28\,\theta R\left(4x\varepsilon/\sigma\right)\frac{\varepsilon}{\sigma} \tag{37}$$

with

$$R(t) = \frac{\left(1 - t + 6t^2\right)^3}{(1-3t)^{3/2}(1-t)^7}, \qquad 0 \le t < \frac{1}{3}, \tag{38}$$

and $|\theta| \le 1$. In particular, in the i.i.d. case, for all $0 \le x = o(\sqrt{n}), n \to \infty$,

$$\left|\mathbb{P}(S_n > x\sigma) - M(x)\inf_{\lambda \ge 0} \mathbb{E} e^{\lambda(S_n - x\sigma)}\right| = O\left(\frac{1}{\sqrt{n}}\inf_{\lambda \ge 0} \mathbb{E} e^{\lambda(S_n - x\sigma)}\right) \tag{39}$$

and thus

$$\frac{\mathbb{P}(S_n > x\sigma)}{M(x)\inf_{\lambda \ge 0} \mathbb{E} e^{\lambda(S_n - x\sigma)}} = 1 + o(1). \tag{40}$$

6.4. A fractional Brownian field indexed by L^2 and a varying Hurst parameter

Participant: Alexandre Richard.

Using structures of Abstract Wiener Spaces and their reproducing kernel Hilbert spaces, we define a fractional Brownian field indexed by a product space $(0, 1/2] \times L^2(T, m)$, where the first coordinate corresponds to the Hurst parameter of fractional Brownian motion. This field encompasses a large class of existing fractional Brownian processes, such as Lévy fractional Brownian motion and multiparameter fractional Brownian motion, and provides a setup for new ones. We prove that it has good incremental variance in both coordinates and derive certain continuity and Hölder regularity properties. Then, we apply these general results to multiparameter and set-indexed processes, which proves the existence of processes with prescribed local Hölder regularity on general indexing collections.

The family of fBm can be considered for the different Hurst parameters as a single Gaussian process indexed by $(h, t) \in (0, 1) \times \mathbb{R}_+$, which is the position we adopt. Besides, the "time" indexing is replaced by any separable L^2 space. We prove that there exists a Gaussian process indexed by $(0, 1/2] \times L^2(T, m)$, with the additional constraint that the variance of its increments is as well behaved as it was on $(0, 1) \times \mathbb{R}_+$, that is, for any compact of L^2, there is a constant $C > 0$ such that for any f in this compact, and any $h, h' \in (0, 1/2)$,

$$\mathbb{E}\left(B_f^h - B_f^{h'}\right)^2 \le C\ (h - h')^2. \tag{41}$$

When looking at the L^2–fBf with a fixed h, we have the following covariance: for each $h \in (0, 1/2]$,

$$k_h : (f, g) \in L^2 \times L^2 \mapsto \frac{1}{2}\left(m(f^2)^{2h} + m(g^2)^{2h} - m(|f-g|^2)^{2h}\right) \ . \tag{42}$$

An important subclass of these processes is formed by processes restricted to indicator functions of subsets of T. In particular, multiparameter when $(T, m) = (\mathbb{R}_+^d, \text{Leb.})$, and more largely set-indexed processes [62],[20] naturally appear and thus motivate generalization *b)*, besides the inherent interest of studying processes over an abstract space.

To define this field, we used fractional operators on the Wiener space W introduced in [56], and first expressed the fractional Brownian field (indexed by $(0, 1/2] \times \mathbb{R}_+$) as a white noise integral over W:

$$\left\{ \int_W \langle \mathcal{K}_h R_h(\cdot, t), w \rangle \ \mathrm{d}\mathbb{B}_w, \ \ (h, t) \in (0, 1/2] \times \mathbb{R}_+ \right\} \ ,$$

The advantage of this approach is to allow the transfer of techniques of calculus on the Wiener space to any other linearly isometric space with the same structure (those spaces are called Abstract Wiener Spaces). Using the separability and reproducing kernel property of the Cameron-Martin spaces built from the kernels $k_h, h \in (0, 1/2]$, we prove the existence of a Brownian field $\{\mathbf{B}_{h,f}, \ \ h \in (0, 1/2], f \in L^2(T, m)\}$ over some probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Some Hilbert space analysis then provides the desired bound (22). Then, we used this to derive a sufficient condition for almost sure continuity of the fractional Brownian field, in terms of metric entropy.

For fixed h, we proved that the h-fractional Brownian motion has the strong local nondeterminism property, which allowed to compute a sharp estimate of its small deviations, that is, for a compact K of L^2:

$$\exp\left(-C \ N(K, d_h, \varepsilon)\right) \leq \mathbb{P}\left(\sup_{f \in K} |\mathbf{B}_f^h| \leq \varepsilon\right) \leq \exp\left(-C^{-1} \ N(K, d_h, \varepsilon)\right) \ ,$$

where $N(K, d_h, \varepsilon)$ is the metric entropy of K, i.e., the minimal number of balls necessary to cover K with d_h-balls (the metric induced by the h-fBm) of radius at most ε.

Finally, we looked at the Hölder regularity of the fBf, when the L^2 indexing collection is restricted to the indicator functions of the rectangles of $\mathbb{R}^d$ (multiparameter processes) or to some indexing collection (in the sense of [62]). This restriction permits to use local Hölder regularity exponents, in the flavour of what was done in [24]. When a regular path $\mathbf{h} : L^2 \to (0, 1/2]$ is specified, this defines a multifractional Brownian field as $\mathbf{B}_f^{\mathbf{h}} = \mathbf{B}_{\mathbf{h}(f), f}$, whose Hölder regularity at each point is proved to equal $\mathbf{h}(f)$ almost surely.

6.5. Self-stabilizing processes

Participants: Xiequan Fan, Jacques Lévy Véhel.

In collaboration with K. Falconer, University of St Andrews.

Self-stabilizing processes are càdlàg processes whose local intensiy of jumpd depend on amplitude. We have investigated two paths to define such processes. The first one is based on a modification of the celebrated Lévy construction of Brownian motion.

The second one starts from a stochastic differentiel equation, and allows one to build Markov processes, a useful feature in applications such as financial modelling [40], [41].

6.6. Multifractal spectra of multistable Lévy motion

Participant: Jacques Lévy Véhel.

In collaboration with R. Le Guével, University of Rennes.

As a follow-up to the work in [34] we have computed the Hausdorf, large deviation, and Legendre multifractal spectra of multistable Lévy motion. It turns out that the shape of the Hausdorf multifractal spectrum is much more complex than could be expected considering the corresponding spectrum of plain Lévy motion. Also, the large deviation spectrum reveals more information on the fine structure of the process than the Hausdorf one, a situation reminiscent of what has already been observed for the model we have developped previously for TCP traffic [2],[39].

6.7. Self-regulating processes for the modelling of geophysical signals

Participant: Jacques Lévy Véhel.

In collaboration with A. Echelard and A. Philippe, University of Nantes.

We have shown that various geophysical signals, and in particular temperature records, can be modelled with self-regulating processes as introduced in [4]. For this purpose, we have used an estimator of the self-regulating function proposed in [44]. Such a modelling allows one to gain further insight on the fine structure of the evolution of temperatures.

6.8. Regularity-preserving signal denoising

Participant: Jacques Lévy Véhel.

In collaboration with A. Echelard.

We have proposed a new wavelet-based method for signal denoising, that allows one to recover the local Hölder regularity of the original signal under weak assumptions [43]. The algotihm is a modification of the well-known wavelet thresholding procedure, where "small" coefficients are not put to zero, but modified in a way governed by the behaviour of large scale coefficients. This will have applications in the frame of our Tandem project on the analysis of radar images.

TOSCA Project-Team

6. New Results

6.1. Probabilistic numerical methods, stochastic modelling and applications

Participants: Mireille Bossy, Nicolas Champagnat, Julien Claisse, Madalina Deaconu, Samuel Herrmann, James Inglis, Antoine Lejay, Sylvain Maire, Sebastian Niklitschek Soto, Denis Talay, Etienne Tanré, Denis Villemonais, Laurent Violeau.

6.1.1. Published works and preprints

- M. Bossy and J-F. Jabir (University of Valparaíso) [29], have proved the well-posedness of a conditional McKean Lagrangian stochastic model, endowed with the specular boundary condition, and further the mean no-permeability condition, in a smooth bounded confinement domain $\mathcal{D}$. This result extends their previous work [48], where the confinement domain was the upper-half plane. The extension of the construction to more general confinement domain exhibits difficulties that we handle by combining stochastic calculus and the analysis of kinetic equations. As a prerequisite for the study of the nonlinear case, we construct a Langevin process confined in $\overline{\mathcal{D}}$ and satisfying the specular boundary condition. We then use PDE techniques to construct the time-marginal densities of the nonlinear process from which we are able to exhibit the conditional McKean Lagrangian stochastic model.
- N. Champagnat studied in collaboration with S. Méléard (Ecole Polytechnique, Palaiseau) and P.-E. Jabin (Univ. of Maryland) adaptive dynamics and evolutionary branching in individual-based models of populations competing for resources, where resources consumption is modelled similarly as for chemostat systems of ODEs [13].
- M. Deaconu and S. Herrmann constructed a new procedure for the simulation of the hitting times of nonlinear boundaries for Bessel processes. This method, called the random walk on moving spheres algorithm, is based on two key properties: first, the explicit distribution of the first hitting time of a particular boundary for the Bessel process; second, the connexion between the Bessel process and the Euclidean norm of a Brownian motion having the same dimension. This result can be applied for the hitting time of a given level for the Cox-Ingersoll-Ross process and thus be used in models arising from finance and neurosciences [15].
- J. Inglis and E. Tanré completed their study with F. Delarue and S. Rubenthaler (Univ. Nice – Sophia Antipolis) on the global solvability of a networked system of integrate-and-fire neurons proposed in the neuroscience literature. To do this it was necessary to obtain some general estimates of the first hitting times of barriers by non-homogeneous processes, which have been collected together separately in [40], http://hal.inria.fr/hal-00870991.
- J. Inglis, in collaboration with O. Faugeras (EPI NeuroMathComp), studied the well-posedness of stochastic neural field equations within a rigorous framework. The deterministic versions of these equations have been used to great success for the macroscopic modeling of brain activity. Their stochastic counterparts are non-trivial SPDEs, due to the presence of a nonlocal operator [26], http://hal.inria.fr/hal-00907555.
- A. Lejay and L. Coutin (Université de Toulouse) have continued their work on the sensitivity of the Itô's map in the context of rough paths [37].
- With L. Coutin (Université de Toulouse), A. Lejay has provided a framework for considering linear rough differential equations [49].
- With A. Kohatsu-Higa (Ritsumeikan University) and K. Yasuda (Hosei University), A. Lejay provided bounds on the weak rate of convergence of the Euler scheme when the drift term is discontinuous [41].

- S. Maire and G. Nguyen have developed a Monte Carlo method to deal with Robin and transmission conditions for elliptic diffusion equations in stratified media. It combines walk on spheres techniques and finite differences [44].
- D. Villemonais worked on the empirical distribution of Fleming-Viot type particle systems. Using couplings with reflected diffusion processes, he proved the uniform tightness of such empirical distributions and deduced the non-degeneracy of the law of diffusion processes conditioned not to hit a boundary [19].
- D. Villemonais proved in [18] a general approximation method for Markov processes conditioned not be killed. The method is based on a mean field interacting particles system which is easy to simulate. The study also details the particular case of time/environment dependent diffusion processes.

6.1.2. Other works in progress

- N. Champagnat and B. Henry work on the long-time behaviour of the frequency spectrum for the Splitting Tree models under the infinitly-many alleles model. Specificaly, they want to study the asymptotic behavior of the largests families in the "supercritical clonal" case. Such results could be applied to design statistical methods to detect positive selection of a gene in a growing population.
- N. Champagnat, D. Ritchie (ORPAILLEUR team, Inria Nancy) and B. Henry work on the design of a stochastic model for the evolution of 3D structures of proteins. Using Kpax algorithm [52], which allow to quantify the evolutionary distance between proteins, their goal is to design a statistical method to infer phylogenetic trees with particle systems methods.
- N. Champagnat and D. Villemonais obtained criterions for existence and uniqueness of quasi-stationary distributions and Q-processes for general absorbed Markov processes. A quasi-stationary distribution is a stationary distribution conditionnally on non-absorbtion, and the Q-process is defined as the original Markov process conditionned to never be absorbed. The criterion that they obtain ensures exponential convergence of the conditionned t-marginal of the process conditionned not to be absorbed at time t, to the quasi-stationary distribution and also the exponential ergodicity of the Q-process. This work is currently being written.
- J. Claisse continued his PhD. under the supervision of N. Champagnat and D. Talay on stochastic control of population dynamics. He completed a finite-horizon optimal control problem on branching–diffusion processes. He also created and studied a hybrid model of tumor growth emphasizing the role of acidity. Key therapeutic targets appear in the model to allow investigation of optimal treatment problems.
- M. Deaconu and S. Herrmann are developing a new algorithm for the simulation of Bessel processes hitting times for non-integer dimensions. The idea is to decompose the dimension into its integer part and its fractional part and use the additivity property for squared Bessel processes. Each simulation step is splitted in two parts: one uses the integer dimension case and the other one considers hitting times of a Bessel process starting from zero.
- M. Deaconu in collaboration with L. Beznea (IMAR Bucarest) and O. Lupaşcu (Université Paris 13 and IMAR Bucarest) studies the connexion between the coagulation/fragmentation phenomena and branching processes.
- J. Inglis and D. Talay are developing a mean-field model of a network of neurons, that contains both a spatial element describing the transmission of a signal along dendrites, as well as non-homogenous weights that represent the strength of the synaptic connections. More generally, this leads to the study of the limiting behavior of non-exchangeable mean-field particle systems.
- J. Inglis and E. Tanré are continuing their collaboration with F. Delarue (Univ. Nice – Sophia Antipolis) by developing approximations to a limiting equation describing the behavior of a large network of neurons all behaving according to the integrate-and-fire model. Both a particle system approximation and an approximation involving delays are considered.
- S. Larnier and A. Lejay have worked on nearshore wave analysis and bathymetry identification through the use of a video installed on the shore [42], [43].

- A. Lejay has continued his work with R. Rebolledo (Pontificia Universidad Católica), S. Torres (Universidad de Valparaíso) and E. Mordecki (Universidad de la República) on the parametric estimation of coefficients of diffusion with discontinuous coefficients.
- S. Maire and I. Dimov (Bulgarian academy of sciences) have introduced a new Monte Carlo method to solve real or complex linear systems of equations. Coupled with sequential Monte Carlo this walk on equations method shows a very fast convergence. A similar method is in progress to solve linear integral equations.
- S. Niklitschek Soto and D. Talay have set up and solved a new martingale problem which has allowed them to get a new stochastic representation for solutions of multi-dimensional diffraction parabolic PDEs with general discontinuous coefficients. One of the main difficulties to overcome has been to identify the proper weighted local time process involved in the stochastic dynamics. This work opens the way to innovating Monte Carlo methods for this class of PDEs.
- P. Guiraud (University of Valparaíso) and E. Tanré study the effect of noise in the phenomenon of spontaneous synchronisation in a network of full connected integrate- and-fire neurons. They detail cases in which the phenomenon of synchronization persists in a noisy environment, cases in which noise permits to accelerate synchronization, and cases in which noise permits to observe synchronization while the noiseless model does not show synchronization. (Math Amsud program SIN)
- L. Capietto worked during his internship under the supervision of O. Faugeras (EPI NEUROMATHCOMP) and E. Tanré on extension of [51], in a context with several populations of homogeneous neurons. They study the limit mean field equation of the membrane potential as the number of neurons increase in a network with correlated synaptic weights.
- E. Tanré, in collaboration with O. Faugeras (EPI NEUROMATHCOMP) and the team Inference and Visual Behavior (IViBe) of Institut de Neurosciences de la Timone (INT), studied the motion of eyes, the phenomena of sacades and micro-saccades when monkeys or humans have to fix the center of a picture during a few minutes. They introduce a stochastic model to describe the typical path of the eyes on the picture and evaluate the link between the characteristics of the artificial pictures and the coefficients of the stochastic model.
- L. Violeau continued his PhD. on *Stochastic Lagrangian Models and Applications to Downscaling in Fluid Dynamics* under the supervision of M. Bossy and A. Rousseau (LEMON team, Inria Sophia Antipolis - Méditerranée). Laurent Violeau has obtained a theoretical rate of convergence of the particle approximation of kinetic conditional McKean-Vlasov stochastic models. This result is the first that explicits the complex relationship between the two sources of spacial errors in such kind of algorithm: the smoothing parameter for the conditional expectation estimator and the number of interacting particles. This theoretical convergence rate was confronted with numerical tests in the case of simplified Lagrangian models that confirm the pertinence of the theoretical bound for the error.
- C. Graham and D. Talay are writing the second volume of their series published by Springer on the Mathematical Foundations of Stochastic Simulations.
- In collaboration with N. Touzi (Ecole Polytechnique), D. Talay is studying stochastic differential equations involving local times with stochastic weights, and extensions of classical notions of viscosity solutions to PDEs whose differential operator has discontinuous coefficients and transmission boundary conditions.

6.2. Financial Mathematics

Participants: Mireille Bossy, Nicolas Champagnat, Paul Charton, Madalina Deaconu, Dalia Ibrahim, Antoine Lejay, Khaled Salhi, Denis Talay, Etienne Tanré.

6.2.1. Published works and preprints

- In collaboration with N. Maïzi (CMA - Mines Paristech) and O. Pourtallier (COPRIN team, Inria Sophia Antipolis - Méditerranée), M. Bossy studied the existence result of a Nash equilibrium between electricity producers selling their production on an electricity market and buying CO2 emission allowances on an auction carbon market. The producers' strategies integrate the coupling of the two markets via the cost functions of the electricity production. The authors set out a clear Nash equilibrium that can be used to compute equilibrium prices on both markets as well as the related electricity produced and CO2 emissions covered [30]
- In addition to the internship of K. Salhi, N. Champagnat, M. Deaconu, and A. Lejay have worked on the use of power law to predict risk in financial markets using data from Euronext NSYE stocks exchanges [33].
- P. Charton submitted an article [35] on the optimal operation of a windfarm equipped with a storage unit.

6.2.2. Other works in progress

- D. Ibrahim, D. Talay and E. Tanré worked on a model coming from technical analysis in finance. They study the Bollinger Bands indicator to detect jumps in the volatility in an extension of classical Black and Scholes models. They evaluate the efficiency of such indicators to detect the random time at which the volatility jump from a *small* value to a *large* one. A paper is being written.
- In collaboration with Victor Reutenauer and Christophe Michel (CA-CIB), D. Talay and E. Tanré worked on a model in financial mathematics including bid-ask spread cost. They study the optimal strategy to hedge an interest rate swap that pays a fixed rate against a floating rate. They present a methodology using a stochastic gradient algorithm to optimize strategies. A paper is being submitted.
- In collaboration with J. Bion-Nadal (Ecole Polytechnique and CNRS), D. Talay introduced a new calibration method based on dynamical risk measures and stochastic control PDEs. A paper is being written.

6.3. Stochastic Analysis

Participants: Nicolas Champagnat, Julien Claisse, Denis Talay.

- N. Champagnat studied in collaboration with P.-E. Jabin (Univ. of Maryland) strong existence and pathwise uniqueness for stochastic differential equations driven by a Brownian motion and with rough coefficients [34]. The method is an extension of the one of [50], which studies well-posedness for deterministic dynamical system. Strong existence and pathwise uniqueness can be proved for example if the drift vector is $L^1(W^{1,1})$ and the diffusion matrix is uniformly elliptic and $L^q(W^{1,p})$ with $2/q + d/p = 1$. This improves the previous conditions of [53].
- J. Claisse and D. Talay studied in collaboration with X. Tan (Univ. of Paris Dauphine) a conditioning argument which is often used to prove the dynamic programming principle [36]. Their study of the literature revealed that previous proofs of this argument are incorrect or incomplete. They provided a rigorous and detailed proof by setting up martingale controlled problems in a original way.